ANNUAL INTERNAL QUALITY ASSESSMENT STATUS REPORT

Name of the School: **School of Chemical Sciences**

Year of Report: **2011-2012**

Part A: **The plan of action chalked out by the IQAC in the beginning of the year towards quality enhancement and the outcome achieved by the end of the year.**

IQAC conceived of integrating contemporary knowledge with the curriculum imparted to the students so that frontiers of the Chemical Sciences are meaningfully explored. The plan of action chalked out to meet this objective relied heavily on modernization of curriculum, organization of National Seminar with lectures and corresponding brain storming sessions and procurement of sophisticated equipments, Consequently, exhaustive revision on curriculum was undertaken to take care of the knowledge gaps and to address the relevant issues and the School has purchased FTIR and UV-Vis. Spectrophotometer. The school successfully organized a National Seminar on the theme entitled **"Emerging Trends in Chemical Sciences"** in 2012 and academic fraternity of entire University was benefited by this exercise.

Part B:

1.	Activities reflecting the goals and objectives of the institution	To explore new horizons of knowledge in chemical sciences and to blend it effectively in academic curricula for overall educational purpose. To fulfill these goals and objectives, we have undertaken following activities. • Rigorous teaching with teaching adds. • Strong emphasis on research activities. • Encouragement to the students to undertake challenging assignments. • Seminar presentation by students.
2.	New academic programmes initiated (UG and PG)	None
3.	Innovations in curricular design and transaction	• Curriculum of M.Sc. Chemistry, Applied Chemistry and Pharmaceutical Chemistry has been substantially revised for session 2011-12 and onwards. • New experiments have been added .
4.	Inter-disciplinary programmes started	In all M.Sc. programmes interdisciplinary papers such as Mathematics for Chemists, Biology for Chemists and Computer Applications have been included
5.	Examination reforms implemented	Semester system is followed in its true spirit . Answer sheets are shown to the students after evaluation.

6.	Candidates qualified NET/SLET/GATE etc.	No of students selected through NET / GATE **:** NET = 02 ; GATE: 01
7.	Initiative towards faculty development programme	Faculty members have interacted with eminent scientists. Prof. B. Vishwanathan, IIT Madras Prof. Deepak Gupta, IIT Kanpur Prof. P. Yogeeshwari, BITS Pilani, Hyderabad Prof. Akhilesh Verma, University of Delhi
8.	Total number of seminars / workshops conducted	The school organized a National Seminar on the theme entitled **"Emerging Trends in Chemical Sciences"** in 2012
9.	Research projects a)Newly implemented: b)Completed:	See **Annexure I** On going : 02 Completed: 06
10.	Patents generated if any	Nil
11.	New collaborative research programmes	See **Annexure II**
12.	Research grants received from various agencies	See **Annexure I**
13.	Details of research scholars	Students with fellowships : 05 Students without fellowship : 18 Rajiv Gandhi National fellowship : 01
14.	Citation index of faculty members and impact factor	See list of publications of faculty members with impact factor. See **Annexure III**
15.	Honors/Awards to the faculty	Prof. Ashok Kumar (in Faculty category)and Mr. Pankaj Patidar (in Student Category) have been awarded by **"Best Science Research Award of MPCST in 2012"**
16.	Internal resources generated	Departmental Fees
17.	Details of departments getting SAP, COSIST (ASSIST) / DST.FIST, etc. assistance/recognition	Rs. 30 lakhs as FIST support from DST
18.	Community services	Faculty , students and non teaching staff participated in plantation activities
19.	Teachers and officers newly recruited	None
20.	Teaching-Non-teaching staff ratio	Ratio : 11: 19 (as per sanctioned posts)
21.	Improvements in the library services	New books with latest titles have been added in the Library.

22.	New books/journals subscribed and their value	Procurement of various standard books has been done from time to time and facility of various International Journals has been provided for all faculty members and Research scholars through Science Direct.
23.	Courses in which student assessment of teachers is introduced and the action taken on student feedback	Student's feedback was analyzed . Overall rating of the faculty members was very good.
24.	Unit cost of education Unit Cost = Total annual expenditure budget (Actual) divided by the number of students enrolled	About Rs. 1.15 Lakh per student
25.	Computerization of administration and the process of admissions and examination results, issue of certificates	• All the results of the semester examination grade sheets are prepared on the computer. • All day to day letters, Dept profiles, data asked from the University are prepared on the computer.
26.	Increase in the infrastructural facilities	New equipments such as FTIR and UV-Vis spectrophotometer have been purchased to augment the research activity of the School and facilities for M.Sc. practical.
27.	Technology up gradation	Networking facility through IT center has been provided to facilitate teaching and research.
28.	Computer and internet access and training to teachers and students	Yes
29.	Financial aid to students	Scholarship to SC/ST students is provided by state Government for M.Sc students.
30.	Activities and support from the Alumni Association	Alumni help the students to find opportunities of research and jobs.
31.	Activities and support from the Parent Teacher Association	None
32.	Health services	Students are provided health centre facility by the University.
33.	Performance in sports activities	Students participated in the sports activity organized by UTD sports association.
34.	Incentives to outstanding Sports persons	None
35.	Student achievements and awards	• Mr. Pankaj Patidar has been awarded by **"Best**

		Science Research Award of MPCST in 2012" • Mr. Sunil Patidar and Mr. Dileep Singh Sisodiya won the award in Quiz competition organized by MPCST in 2012.
36.	Activities of the Guidance and Counseling unit	Faculty members guide the students from time to time on various issues including research opportunities and preparation for NET/ GATE exam.
37.	Placement services provided to students	Faculty members guide the students for job opportunities in academic Institutions and Industries.
38.	Development programmes for non-teaching staff	None
39.	Healthy practices of the institution	• Regular and quality teaching • Active participation in research activity
40.	Linkages developed with National/International, Academic/Research bodies	See **Annexure II**
41.	Any other relevant information the institution wishes to add	School's mission is to provide high quality education and training for high flying careers in Chemical Sciences. Our distinguishing features are: • Theoretical and practical knowledge of Instrumental Techniques. • Interpretation of various types of spectra. Nuclear Magnetic Resonance (NMR) Electron Spin Resonance (ESR), Infrared (IR), Ultraviolet-Visible (UV-Visible), Mössbauer, Mass Spectrometry. • The strength of the School has been and continues to be excellence in research and teaching. • The faculty is extremely well qualified and motivated with a strong commitment to research.

(PART – C)

Detail the plans of the institution for the next year:

Yearly plan: 2012 -2013

Curriculum

- It is planned to increase the diversity in spectral interpretation w.r.t. new examples and relevant patterns.

- The syllabus is revised generally in the beginning of the session to include recent advancements.

Strategies of Teaching Learning

Use of teaching aids to be encouraged and novel methods of learning such as quiz to be adopted as and when applicable.

Student Feedback System Design

Students' feedback about the School , faculty members and the curriculum would be practiced as per IQAC design.

Collection of Feedback and its Analysis: Format of Analysis

Feedback will be collected by Dec 2012 and May 2013 and will be analyzed by faculty members. The overall report will be prepared and necessary improvements will be done for coming year.

Improvement Plan

Infrastructure

New building for School of Chemical Sciences needs to be constructed on high priority basis.

Research Activities and Promotion

- Faculty members would be encouraged to participate in seminars and conferences
- Collaborative research activities will be promoted.

Name and Signature of the Coordinator QAC

Name and Signature of the HEAD

Annexure I

Details of research grant received from different agencies during the last five years: 2007-2012

Name of the Investigator	Title of the project and duration	Status	Amount sanctioned	Funding agency
Dr. R. Prasad	Surface and catalytic studies of nanocrystalline and nanoporous metal oxides	Completed	Rs.3,06,000/-	CSR-CRS
	Studies of few catalytic vapourphase alkylation and cyclization reactions.	Completed	Rs. 7,64,800/-	UGC
Dr. Ashok Kumar	Synergistic extraction and spectrophotometric deter-mination of toxic metal ions and lanthanides at trace level by chromogenic substituted calix(n) arenes.	Completed	Rs. 10,46,000/-	CSIR
	Synergistic extraction and stripping voltammetric determination of toxic metal ions and lanthanides at trace level.	Completed	Rs. 17,00,000/-	DST
Dr. H.P.S. Chauhan	Synthetic, Spectroscopic, Thermal and Biochemical Studies on some Group 14 (Si, Ge and Sn) and Group 15 (As, Sb and Bi) Metal and Organometallic Complexes with some sulphur and/or Oxygen Donor Organic Ligands	Completed	Rs.4,11,100/-	UGC
Dr Pratibha Sharma	Design, Synthesis, Electrochemical Studies and Evaluation of Therapeutic Potential of Purines and Benzimadazoles Through Quantitative Structure - Activity Relationship	Completed	Rs.14,94,000/-	DRDO
Dr. R. Prasad	Quantum Mechanical and Molecular Mechanics Computation of few molecules, Reactions and Nano matwerials	Ongoing	Rs. 2,95,000	MPCST, Bhopal
Dr. H.P. S. Chauhan	Group 15 Metal and Organometallic Derivatives with Mixed Sulphur and/or Oxygen Donor Ligands: Synthesis and Characterization: Thermal and Biochemical Studies	Ongoing	Rs. 8,04,800	UGC , New Delhi

Annexure II

International Collaboration of the Professors:

Dr. K.K. Pandey

Collaborative Research work with European and American Scientists

1. Prof. H.W. Roesky
   Institute of Inorganic Chemistry
   University of Gottingen, Germany

2. Prof. G.M. Sheldrick
   Institute of Inorganic Chemistry
   University of Gottingen, Germany

3. Prof. B. Krebs
   Institute of Inorganic Chemistry
   University of Munster, Germany

4. Prof. J.W. Bats
   Institute of Crystallography and Mineralogy
   University of Frankfurt, Germany

5. Prof. G. Frenking
   Faculty of Chemistry
   University of Marburg, Germany

6. Prof. Philip P. Power
   Department of Chemistry
   University of California Davis, USA

7. Prof. Agusti Lledos
   Department of Chemistry
   University of Autonoma Barcelona, Spain

8. Prof. F. Maseras
   Institute of Chemical Research of Cataonia (ICIQ)
   Tarragona, Spain

9. Dr. D.G. Musaev

Director
Emerson Center for Scientific Computation
Emory University, Atlanta, Georgia, USA

10. Prof. D.C. Liotta
    Editor: J. Medicine Chem. Letters (American Chemical Society, USA)
    Department of Chemistry
    Emory University, Atlanta, Georgia, USA

11. Prof. Simon Aldridge
    Department of Chemistry
    Oxford University, UK

12. Prof. Holger Braunschweig
    Department of Chemistry
    University of Würzburg, Germany

13. Prof. Alexander C. Filippou
    Department of Chemistry
    University of Bonn, Germany

Annexure III

SCHOOL OF CHEMICAL SCIENCES
DEVI AHILYA UNIVERSITY INDORE

PUBLICATION During the Period 2007- July 2012

DR. KRISHNA K. PANDEY

1. Energy Analysis of Metal-Metal Bonding in [RM-MR] (M = Zn, Cd, Hg; R = CH_3, SiH_3, GeH_3, C_5H_5, C_5Me_5]
   Krishna K. Pandey
   J. Organomet. Chem. 692 (2007) 1058-1063.
   Impact Factor: 2.384

2. Structure and Coordinate Bonding Nature of the Rhenium-σ-borane complexes
   Krishna K. Pandey
   J. Mol. Struct. (THEOCHEM) 807 (2007) 61-66.
   Impact Factor: 1.288

3. Structure and coordinate bonding nature of the manganese-σ-borane complexes
   Krishna K. Pandey
   J. Organomet. Chem. 2007, 692, 1997-2005.
   Impact Factor: 2.384

4. Transition Metal-Carbon Complexes. A Theoretical Study
   Andreas Krapp, Krishna K. Pandey and Gernot Frenking
   J. Am. Chem. Soc. 129 (2007) 7596-7610.
   Impact Factor: 9.099

5. Structure and energy decomposition analysis of metal-metal bonding in [PhM-MPh] and [ClM-MCl] (M = Zn, Cd, Hg)
   K.K. Pandey
   J. Mol. Struct. (THEOCHEM) 823 (2007) 59-64.
   Impact Factor: 1.288

6. Stretched σ-borane complexes of rhodium: A theoretical study
   K.K. Pandey
   Inorg. Chem. Commun. 11 (2008) 288..
   Impact Factor: 1.972

7. σ-Borane complexes of nickel, palladium and platinum. A theoretical study
   K.K. Pandey
   J. Mol. Struct. (THEOCHEM) 855 (2008) 18.
   Impact Factor: 1.288

8. Mixed-ligand Ru(II) complexes with 2,2'-bipyridine and tetradentate Schiff bases ligands: Synthesis, physico-chemical study, DFT analysis, electrochemical and Na binding properties
   L. Mishra, R. Prajapati, K.K. Pandey
   Spectrochimica Acta (A): Molecular and Bimolecular Spectroscoscopy 70 (2008) 79-85.
   Impact Factor: 1.952

9. Transition Metal sigma-borane complexes
   K.K. Pandey
   Coord. Chem. Revs. 253 (2009) 37.
   Impact Factor: 12.110

10. Linear M≡E-Me Versus Bent M-E-Me: Bonding Analysis in Heavier Metal- ylidyne Complexes [(Cp)$(CO)_2$M≡EMe] and Metallo-ylidenes [(Cp)$(CO)_3$M-EMe] (M = Cr, Mo, W; E = Si, Ge, Sn, Pb)
    Krishna K. Pandey and Agustí Lledós
    Inorg. Chem. 48 (2009) 2748-2759.
    Impact Factor: 4.601

11. The Nature of M-B Versus M=B Bonds in Cationic Terminal Borylene Complexes: Structure and Energy Analysis in the Borylene Complexes $[(\eta^5\text{-}C_5H_5)(CO)_2M\{B(\eta^5\text{-}C_5Me_5)\}]^+$, $[(\eta^5\text{-}C_5H_5)(CO)_2M(BMes)]^+$, and $[(\eta^5\text{-}C_5H_5)(CO)_2M(BNMe_2)]^+$ (M = Fe, Ru, Os)
    Krishna K. Pandey, Agusti Lledos and Feliu Maseras
    Organometallics 28 (2009) 6442-6449.
    Impact Factor: 3.963

12. Structure and Bonding Energy Analysis of Cobalt, Rhodium and Iridium Borylene Complexes $[(\eta^5\text{-}C_5H_5)(CO)M(BNX_2)]$ (X = Me, SiH_3, $SiMe_3$) and $[(\eta^5\text{-}C_5H_5)(PMe_3)M\{BN(SiH_3)_2)]$ (M = Co, Rh, Ir)
    Krishna K. Pandey and Djamaladdin G. Musaev
    Organometallics 29 (2010) 142-148.
    Impact Factor: 3.963

13. Linear versus bent bonding in metal-phosphinidene complexes: Theoretical studies of the electrophilic phosphinidene complexes $[(\eta^5\text{-}C_5H_5)(CO)_2M(PMe)]^+$, $[(\eta^5\text{-}C_5H_5)(CO)_3M(PMe)]^+$ (M = Cr, Mo, W)
    Krishna K. Pandey and Agusti Lledos
    J. Organomet. Chem. 695 (2010) 206-214.
    Impact Factor: 2.384

14. Computational Studies of Transition Metal Selectivity of Octapeptide Repeat Region of Prion Protein (PrP)
    Krishna K. Pandey, James P. Snyder, Dennis C. Liotta and Djamaladdin G. Musaev
    J. Phys. Chem. A 114 (2010) 1127-1135.
    Impact Factor: 2.946

15. New ruthenium(II) thiolato complexes: Synthesis, reactivity, spectral, structural and DFT studies
    Sudhakar D. Dwivedi, Santosh K. Dubey, Ashish K. Singh, Krishna K. Pandey and Daya S. Pandey
    Inorg. Chim. Acta 363 (2010) 2095-2103.
    Impact Factor: 1.846

16. Structure and Bonding Energy Analysis of M-Ga Bonds in Dihalogallyl Complexes Trans-$[X(PMe_3)_2M(GaX_2)]$ (M = Ni, Pd, Pt; X = Cl, Br, I)
    Krishna K. Pandey, Pankaj Patidar, Holger Braunschweig
    Inorg. Chem. 49 (2010) 6994-7000.
    Impact Factor: 4.601

17. Nature of M-Ga Bonds in Dihalogallyl Complexes $(\eta^5\text{-}C_5H_5)(Me_3P)_2M(GaX_2)$ (M = Fe, Ru, Os) and $(\eta^5\text{-}C_5H_5)(OC)_2M(GaX_2)$ (X = Cl, Br, I): A DFT Study
    Krishna K. Pandey, Pankaj Patidar, Simon Aldridge
    J. Phys. Chem. A 114, 2010, 12099-12105.
    Impact Factor: 2.946

18. Nature of Bonding in Terminal Borylene, Alylene and Gallylene complexes of Vanadium and Niobium $[(\eta^5\text{-}C_5H_5)(CO)_3M(ENR_2)]$ (M = V, Nb; E = B, Al, Ga; R = CH_3, SiH_3, CMe_3, $SiMe_3$): A DFT Study
    Krishna K. Pandey, Holger Braunschweig, Agusti. Lledós
    Inorg. Chem. 50 (2011) 1402-1410.
    Impact Factor: 4.601

19. DFT Study on the Alkylborylene and Haloborylene Complexes of Manganese and Rhenium: Structure and Bonding Energy Analysis in $[(\eta^5\text{-}C_5H_5)(CO)_2M(BR)]$ and $[(\eta^5\text{-}C_5H_5)(CO)_2M(BX)]$ (M = Mn, Re; R = Me, Et, *i*Pr, *t*Bu; X = F, Cl, Br, I)
    Krishna K. Pandey, Holger Braunschweig, Rian D. Dewhurst
    Eur. J. Inorg. Chem. 2011, 2045-2056
    Impact Factor: 3.049

20. Unexpected Generation of Diastereomers by Double Diboration of a Dialkyne
    F. Bauer, H. Braunschweig, K. Gruß, Christoph Lambert, Krishna K. Pandey, K. Radacki, D. Reitzenstein
    Chem. Eur. J. 17 (2011) 5230-5233.
    Impact Factor: 5.925

21. Nature of M-Ga Bonds in Cationic Metal-Gallylene Complexes of Iron, Ruthenium and Osmium $[(\eta^5\text{-}C_5H_5)(L)_2M(GaX)]^+$. A Theoretical Study
    Krishna K. Pandey, Simon Aldridge
    Inorg. Chem. 50 (2011) 1798-1807.
    Impact Factor: 4.601

22. Nature of M-Bi bonds in dihalobismuth complexes of nickel, palladium and platinum trans-[$X(PMe_3)M(BiX_2)$] (M = Ni, Pd, Pt; X = Cl, Br, I)
Krishna K. Pandey
Comput. Theoret. Chem. 967 (2011) 140-146.
Impact Factor: 1.288

23. Nature of M-E bonds in metallosilylenes, germylenes, stannylenes and plumbylenes [$(\eta^5\text{-}C_5H_5)(Me_3P)(H)_2M(EPh)$] (M = Fe, Ru, Os; E = Si, Ge, Sn, Pb)
Krishna K. Pandey, Philip P. Power
Organometallics 30 (2011) 3353-3361
Impact Factor: 3.963

24. Structure and bonding energy analysis of cationic metal-ylyne complexes of molybdenum and tungsten $[(MeCN)(PMe_3)_4M{\equiv}EMes]^+$ (M = Mo, W; E = Si, Ge, Sn, Pb): A Theoretical Study
Krishna K. Pandey, Pankaj Patidar, Philip P. Power
Inorg. Chem. 50 (2011) 7080-7089
Impact Factor: 4.601

25. Structure and bonding analysis of dimethylgallyl complexes of iron, ruthenium and osmium [$(\eta^5\text{-}C_5H_5)(CO)_2M(GaMe_2)$] and [$(\eta^5\text{-}C_5H_5)(Me_3P)_2M(GaMe_2)$]
Krishna K. Pandey
J. Phys. Chem. A 115 (2011) 8578-8585.
Impact Factor: 2.946

26. Structure and bonding in haloarylgallyl complexes of iron, ruthenium and osmium [$(\eta^5\text{-}C_5H_5)(CO)_2M\{Ga(X)(Ph)\}$]: A theoretical study
Krishna K. Pandey, Pankaj Patidar
J. Organomet. Chem. 696 (2011) 3536-3542.
Impact Factor: 2.384

27. Bis(borylene) Complexes of Cobalt, Rhodium, and Iridium [$(\boldsymbol{\eta}^5\text{-}C_5H_5)M(BNX_2)_2$] (X = Me, SiH_3, $SiMe_3$): A Bonding Analysis
Krishna K. Pandey
Organometallics 30 (2011) 5851- 5858.
Impact Factor: 3.963

28. Structure and bonding analysis of dihalogallyl and dimethylgallyl complexes of molybdenum and tungsten [$(\eta^5\text{-}C_5H_5)(CO)_3M(GaX_2)$] (M = Mo, W; X = Cl, Br, I, Me): A Theoretical Study
Krishna K. Pandey
Comput. Theoret. Chem. 973 (2011) 13-19.
Impact Factor: 1.288

29. The nature of M-Ga in metal(I) gallyl complexes of copper, silver and gold: A Theoretical study
    Krishna K. Pandey
    J. Organomet. Chem. 701 (2012) 75-79
    Impact Factor: 2.384

30. Theoretical investigation of M≡E bonds in transition metaleylidyne complexes trans-[$H(PMe_3)_4M{\equiv}ER$] (M = Mo, W; E = Si, Ge, Sn, Pb; R = Mes, Xylyl)
    Krishna K. Pandey, Pankaj Patidar
    J. Organomet. Chem. 702 (2012) 59-66
    Impact Factor: 2.384

31. Structure and bonding analysis in dihalobismuth complexes of iron, ruthenium and osmium [$(\eta^5\text{-}C_5H_5)(CO)_2M(BiX_2)$]: A theoretical Study
    Krishna K. Pandey, Pankaj Patidar, Pradeep Tiwari
    Polyhedron 34 (2012) 84-91.
    Impact Factor: 2.057

32. What is the best bonding model of the (σ-H-BR) species bound to a transition metal: Bonding analysis in complexes [$(H)_2Cl(PMe_3)_2M$(σ-H-BR)] (M = Fe, Ru, Os)
    Krishna K. Pandey
    Dalton Trans. 41 (2012) 3278-3286.
    Impact Factor: 3.840

33. Structure and bonding analysis of dimethylgallyl complexes of cobalt, rhodium and Iridium [$Me(PMe_3)_2(Me_3GaCl)M(GaMe_2)$] (M = Co, Rh, Ir) and [$Me(PMe_3)_2ClIr(GaMe_2)$] : A theoretical study
    Krishna K. Pandey
    J. Organomet. Chem. 710 (2012) 6-11.
    Impact Factor: 2.384

34. Theoretical investigation of triple bond in molybdenum complexes trans-[$X(PMe_3)_4Mo{\equiv}E(Mes)$] (X = F, Cl, Br, I; E = Si, Ge, Sn, Pb): A DFT study
    Krishna K. Pandey, Pankaj Patidar
    Polyhedron 37 (2012) 85-93.
    Impact Factor: 2.057

35. A theoretical study of the bonding and charge distribution in cationic group 8 metal borylene and alylene complexes: Consequences for complex stability and reactivity
    Krishna K. Pandey
    Polyhedron, 43 (2012) 131-139.
    Impact Factor: 2.057

36. Bonding energy analysis in cationic borylene complexes of palladium and platinum: A theoretical study
Krishna. K. Pandey
Polyhedron 2012 Article in Press, DOI: 10.1016/j.poly.2012.04.005
Impact Factor: 2.057

37. The Nature of Mo≡E Bonds: Structure and Bonding Analysis of the Molybdenum-Ylidyne Complexes Trans-[$X(dmpe)_2Mo{\equiv}E(\eta^1\text{-}C_5H_5)$] (E = Si, Ge, Sn, Pb; X = H, Cl, Br, I, CN)
Krishna K. Pandey, Pankaj Patidar, Alexander C. Filippou
Inorg. Chem. 2012 Accepted.
Impact Factor: 4.601

DR. R. PRASAD

1. Synthesis of ethylene carbonate from cyclocondensation of ethylene glycol and urea over $ZnO.Cr_2O_3$catalyst system controlled by co-precipitation method.
Sheenu Bhadauria, Samidha Sexana, Rajandra Prasad, Prabhakar Sharma, Reena Dwivedi.
Eur. J Chem., 3, (2012) 235

2. Microwave assisted synthesis of tetragonal nanocrystalline zirconia Nanoparticles
Reena Dwivedi[a], Anjali Maurya[b], R Prasad[a] and K S Bartwal.
Journal of Alloys and Compounds, 509 (2011) 6848–6851. Impact Factor:2.28

3. Recent Progress in Non-linear Optical Material, Syntheses, Characterization and Geometry Optimization of Dicinnamalacetone
Sheenu Bhadauria, Malyaj Das, Reena Dwivedi**.** Scholars Research Library 2011, 2 (2):36-44

4. Effect of microwave on distribution of Zr4+ and Ti4+ during sol-gel synthesis of ZrTiO4 nanoparticles.
Reena Dwivedi, Akrati Verma, R. Prasad, K.S. Bartwal
Optical Materials. Page ?
Impact Factor:2.02

5. Rigid thermosetting liquid moulding resin from sunflower oil
Navneet Hardia, P. L. Gupta, R.Dwivedi, Samidha Saxena, R. Prasad
Indian journal of Chemical technology, 18, 271-276, 2011.
Impact Factor: 0.267

6. Recent Progress in Non-linear Optical Material, Syntheses, Characterization and Geometry Optimization of Dicinnamalacetone
Sheenu Bhadauria, Samidha Sexana, Rajandra Prasad Reena Dwivedi.
Scholars Research Library 2011, 2 (2):36-44.

7. Kinetics studies and mechanism evolution of the epoxidation of styrene over nanoporous Au doped TS-1
Samidha Saxena, Reena Dwivedi, Sheenu Bhadauria, V. R. Chumbhale and R. Prasad
Details of Publications?
Impact Factor :0.441

8. Vapour Phase Catalytic Synthesis of 2-methylpyrazine over nanocrystalline Ferrite catalyst
Joyjit Basak, Navneet Hardia, Samidha Saxena, Rajeev Dixit, Reena Dwivedi, Sheenu Bhadauria and R.Prasad
Industrial & Engineering Chemistry Research, 2007**. (Details of publicized paprer)**
Impact Factor:2.3

9. Ammoximation of Cyclohexanone over nanoporous TS-1 using UHP as an Oxidant
S. Saxena, J. Basak, N. Hardia, R. Dixit, S. Bhadauria, R. Dwivedi,
R. Prasad, A Soni, G S Okram, A Gupta
Chemical Engineering Journal, 132 **(2007)** 61-66.
Impact Factor: 3.461

10. Structural and catalytic properties of $Zn_{1-x}Cu_xFe_2O_4$ nanoparticles
M. Banerjee, N. Verma, R. Prasad
J. Mater. Sci 42 **(2007)** 1883-1837.
Impact Factor:2.015

DR. ASHOK KUMAR

1. QSAR modeling of synthesized 3-(1,3-benzothiazol-2-yl-2-phenyl quinazolin-4-(3H) ones asotent antibacterial agent
Ashok Kumar, Pratibha Sharma, Prerna Kumari, Jitendra Singh and M. P. Kaushik
Medicinal Chemistry Research, (Springer) 21, 1136–1148 (2012)
(Impact factor 1.271)

2. Synthesis and exploration of QSAR model of 2-methyl-3-[2-(2-methylprop-1-en-1-yl)-1*H*-benzimidazol-1-yl]pyrimido[1,2-a]benzimidazol-4(3*H*)-one as potential antibacterial agents
Pratibha Sharma, **Ashok Kumar**, Manisha Sharma, Jitendra Singh, Prabal Bandyopadhyay, Manisha Sathe, & M. P. Kaushik
Journal of Enzyme Inhibition and Medicinal Chemistry, 27(2), 294-301 (2012)
(Impact factor 1.617)

3. Exploration of antimicrobial and antioxidant potential of newly synthesized 2,3-disubstituted quinazoline-4(3H)-ones
Ashok Kumar, Pratibha Sharma, Prerna Kumari and Bhagwan Lal Kalal
Bioorg. Med. Chem. Lett. **(Elsevier)** 21, 4353-4357 (2011)
(Impact factor 2.554)

4. Methyl-2-(4-methylphenyl)-2H-azirine-3-carboxylate as Dienophile in Hetero Diels Alder Cycloaddition: A DFT approach
   Pratibha Sharma, **Ashok Kumar**, and Vinita Sahu
   Letters in Organic Chemistry, 8, 132-137 (2011)
   (Impact factor 0.822)

5. Theoretical Evaluation of Global and Local Electrophilicity Patterns to Characterize Hetero-Diels-Alder Cycloaddition of Three-Membered 2H-Azirine Ring System
   Pratibha Sharma, **Ashok Kumar**, and Vinita Sahu
   Journal of Physical Chemistry A (**ACS Publication**) 114, 1032–1038 (2010)
   (Impact factor 2.946)

6. A novel approach to the synthesis of 1,2,3-triazoles and their QSAR studies
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