

DEPARTMENT OF CHEMISTRY
BASIC SCIENTIFIC RESEARCH - UGC

1. UTILIZATION PATTERN OF THE THREE INSTALLMENTS OF BSR-INFRASTRUCTURE GRANT
2. FURTHER INSTALLMENT JUSTIFICATION

1. OUTPUT OF THE UTILIZATION OF THE THREE INSTALLMENTS OF BSR-INFRASTRUCTURE GRANT

- ❖ At a time when the students lack interest towards basic science and prefer professional courses, this fund is a boon to attract the students for science in general and chemistry in particular. The assets acquired out of B S R funds have definitely improved the quality of science education as the students are exposed to experiential learning and get hands on experience on state of art, instruments used for research at UG level.
- ❖ Thus, this fund has helped to strengthen the infrastructure and to carryout research projects. This is testified by the list of the projects given below that were carried out by our UG students.

1. Analysis of soft drinks.
2. Application of L-proline as highly efficient organo-catalyst for the synthesis of quinoxalines.
3. Soy milk a better alternative for lactose intolerance.
4. Preparation of bio-diesel from used and unused sunflower oil.
5. Physicochemical characteristics of ground water around Madurai town.
6. Synthesis of Fe^{3+} complexes.
7. Eco waste as corrosion inhibitor for carbon steel in aqueous chloride ion environment.
8. Environmental studies- Estimation of atmospheric carbon dioxide in different localities.
9. Kinetic studies on oxidation of citric acid using permonosulphate.
10. Comparative study of various antacids.
11. Synthesis characterization of Copper anthranilate complex.
12. Analysis of different brands of shampoo.
13. Analysis of extent of unsaturation based on Iodine value in various cooking oils.
14. Waste water treatment of chemistry lab of our College.
15. Analysis of alkalinity in various antacids.

16. Comparison of acetic acid content in home-made and synthetic vinegar and analysis of fresh fruit juices.
17. Analysis of different brands of soap.
18. Synthesis of bio-diesel from used oil and Jatropha plants.
19. 19 Synthesis and characterization of glycinate complex of copper.
20. Estimation of Vitamin C content in lemon.
21. Synthesis and stereochemistry of 2,6-dibenzoyl-3,5-diphenyl-4-cyano-4-phenylthiane-1,1-dioxide.
22. Kinetics of decomposition of peroxomonosulphate by Ni²⁺ in acid medium.
23. MW assisted solvent free synthesis of some 2,6-dibenzoyl-3,5-diphenyl-4,4-diethoxycarbonylthane-1,1-dioxide.
24. An unusual cleavage of α,β -unsaturated olefinic functionality in 2,2'-sulfonylbis-1,3-diarylprop-2-en-1-ones by aniline under MW condition.
25. Synthesis of some 2,2,thiobis-(1,3-diarylprop-2-en-1-ones).
26. Solvent free synthesis of some 2,6-diaroyltetrahydro-1,4-thiazine.
27. MW assisted synthesis of 2,6-diaroyl-3,5-diaryl-4,4-diacetylthiane1,1-dioxide
28. A synthesis of 2,6-diaroyl-3,5-diaryl-1,4-thiazine-1,1-dioxide under MW irradiation.
29. Solvent free synthesis of some 2,6-dibenzoyl-3,5-diphenyl-4,4-diethoxycarbonylthiane1,1-dioxide.
30. Synthesis of multisubstituted tetrahydrofuran.
31. Reaction of 2,2'sulfonylbis1,3-diarylprop-2en-1-one with acetylacetone.
32. Synthesis and characterization of copper complex bearing Schiff base ligands.

2. JUSTIFICATION

BUDGET (2011 - 2012)

S. No.	Items	Amount (₹)
1.	Network Product	15,000
2.	Work Station	2,05,000
3.	Client Terminals	1,74,000
4.	Working table and furniture	1,00,000

5.	UPS	2,10,800
6.	Polarimeter -2 Nos.	60,000
7.	Electronic Balance	50,000
Total		8,14,800

Justification for items 1-5.

Cheminformatics is an IT based applied branch of chemistry, which is a globally an emerging field especially in in-silico drug designing. Chemoinformatics is the mixing of the information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and optimization. The primary application of cheminformatics is in the storage, indexing and search of information relating to compounds. Cheminformatics can also be applied to data analysis for various industries like paper and pulp, dyes and such allied industries.

If a cheminformatics lab is established, a paper on cheminformatics can be introduced at UG level, to motivate the students to take up research. An UG degree in Chemistry with knowledge of cheminformatics provides job opportunities in Pharma Labs and Pharmaceutical companies. This paper can also be offered as an interdepartmental option to students of Physics, Biology and IT. Thus it is proposed to upgrade the infrastructure of laboratory by installing cheminformatics lab.

It also enables the chemistry students to become specialized in chemistry related softwares such as Chemdraw, Sigma-plot, Turbomole etc. Using this facility, UG students can be trained in solving chemistry problems and drawing the graphs with regression analysis for physical chemistry experiments.

Justification for Polarimeter (item 6):

It is used to measure specific rotation of optically active compounds , to follow the kinetics of chemical reactions and to distinguish between optical isomers .

Justification for Electronic Balance (item 7):

It is used to weigh the substances accurately upto 0.1 mg which is required for quantitative analysis.

RESEARCH OUTPUT OF THE DEPARTMENT

1. Research publications:

S. No.	Journal Name	Month/Year	Vol. No.	Issue No.
1.	Synth. Commun.	2009	39	2776
2.	Phosphorus, Sulfur And Silicon	2009	184	-

3.	Tetrahedron	2007	63	2980
4.	Indian Journal of chemical technology	2007	14	71
5.	Journal of Hazardous Materials	2008	147	906
6.	Catalysis Letters	209	132	259
7.	Applied Clay Science	2007	37	193
8.	Journal of Chemical Technology Bio Technology	2008	82	253
9.	Catalysis Letters	2008	120	56
10.	Chinese Journal of Catalysis	2008	29	1202
11.	Asian Journal of Chemistry	2008	20	6
12.	Asian Journal of Chemistry	2008	20	4
13.	International Journal of Chemical Kinetics	2006	-	6-10

2. Major & Minor Projects:

Minor/Major Project/Any other	Funding Agency	Grant Received (₹)	Principal Investigator & Co investigators	Period & Duration
1. Major Project	UGC	6,20,000	Dr. S. Renuga & Dr. M.Gnanadeebam	2006-09
2. Minor Project	UGC	79,000	Dr. L. Latha Kannan	2007-09
3. Minor Project	UGC	60,000	Mrs. S. Selvarani	2006-08
4. Minor Project	UGC	60,000	Mrs. B. Medona	2006-08

3. Chem. informatics lab will be used for the UG students to take up projects under the following topics

- ◆ Molecular Modelling
- ◆ Docking
- ◆ Binding of drugs on biomolecules
- ◆ Drug designing
- ◆ Computational chemistry
- ◆ QSAR studies