Annexure – VIII
UNIVERSITY GRANTS COMMISSION
WESTERN REGIONAL OFFICE
GANESHKHIND, PUNE – 411 007.

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

1. NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATOR : Nirwan R. S. , M.S.G. College,

   Malegaon Camp, Malegaon.

2. NAME AND ADDRESS OF THE INSTITUTION: Mahatma Gandhi Vidyamandir's Maharaja Sayajirao Gaikwad College, Malegaon Camp, Malegaon.

3. UGC APPROVAL NO. AND DATE: No. F. 47-1126/14 (SC/ 72/WRO) XII plan1

4. DATE OF IMPLEMENTATION: March 2017

5. TENURE OF THE PROJECT: Two Years

6. TOTAL GRANT ALLOCATED: 415000/-

7. TOTAL GRANT RECEIVED: 290000/-

8. FINAL EXPENDITURE: **315525.00**-(In Word **Three Lakh Fifteen Thousand Five Hundred Twenty Five only**).

9. TITLE OF THE PROJECT: "Synthesis. Characterization and DFT Study of Some Heterocyclic Compound"

10. OBJECTIVES OF THE PROJECT. To synthesize new heterocyclic compounds .

11. WHETHER OBJECTIVES WERE ACHIEVED: Yes
    (GIVE DETAILS)

12. ACHIEVEMENTS FROM THE PROJECT. New heterocyclic compounds are synthesized.

13. SUMMARY OF THE FINDINGS.: (IN 500 WORDS)

Synthesis of various substituted chalcones by Claisen-Schmidt condensation between aldehydes and substituted o- hydroxyacetophenones using alc. KOH at room temperature stirring for 24 hours. and these chalcones were used to synthesize flavones using DMSO/I2. Substituted flavones were synthesized and characterized by elemental analysis, U.V., IR, ^{1}H NMR and Mass spectroscopy. The synthesized compounds were evaluated for their antibacterial activity against *Escherichia Coli, P. aeruginosa, S. Epidermidis* and *B. Subtilis*. All the flavones showed moderate to good activity.

These flavones were optimized by using DFT method with B3LYP hybrid functional and ab initio (HF & MP2) methods using 6-311++G(d,p) basis set. The spectroscopic properties (UV, IR, ^{1}H NMR) were computed for the optimized geometries at the same level of theory. Geometrical parameters such as Mullikan atomic charges, bond length and bond angles were calculated. Thermodynamic parameters such as energy, heat capacity, entropy, vibrational energy, zero point vibrational energy, rotational constants and dipole moment were calculated. The HOMO, LUMO energy gap was also calculated. Computed values have been analyzed and their characterization was made with the help of Gauss View visualization program utilizing the data obtained from the Gaussian 09W calculation. The overall conclusion is that the gauge independent atomic orbital (GIAO) method with DFT/B3LYP/6-311++G(d,p) level of theory predicted ^{1}H NMR chemical shifts shows good correlation with experimental data. Experimentally observed UV have lower λmax than theoretically predicted. The DFT/B3LYP method shows a very good agreement with experimental stretching vibrations of C-H, C=O, C=C, C-O and C-Cl than MP2 and HF.

14. CONTRIBUTION TO THE SOCIETY: Required more research on these compounds

(GIVE DETAILS)

15. WHETHER ANY PH.D. ENROLLED/PRODUCED. : **No**
OUT OF THE PROJECT

16. NO. OF PUBLICATIONS OUT OF THE PROJECT. **.(04) Four.**
(PLEASE ATTACH RE-PRINTS)

(PRINCIPAL INVESTIGATOR) **(REGISTRAR/PRINCIPAL SIGNATURE & SEAL)**