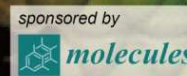




# 19th International Electronic Conference on Synthetic Organic Chemistry

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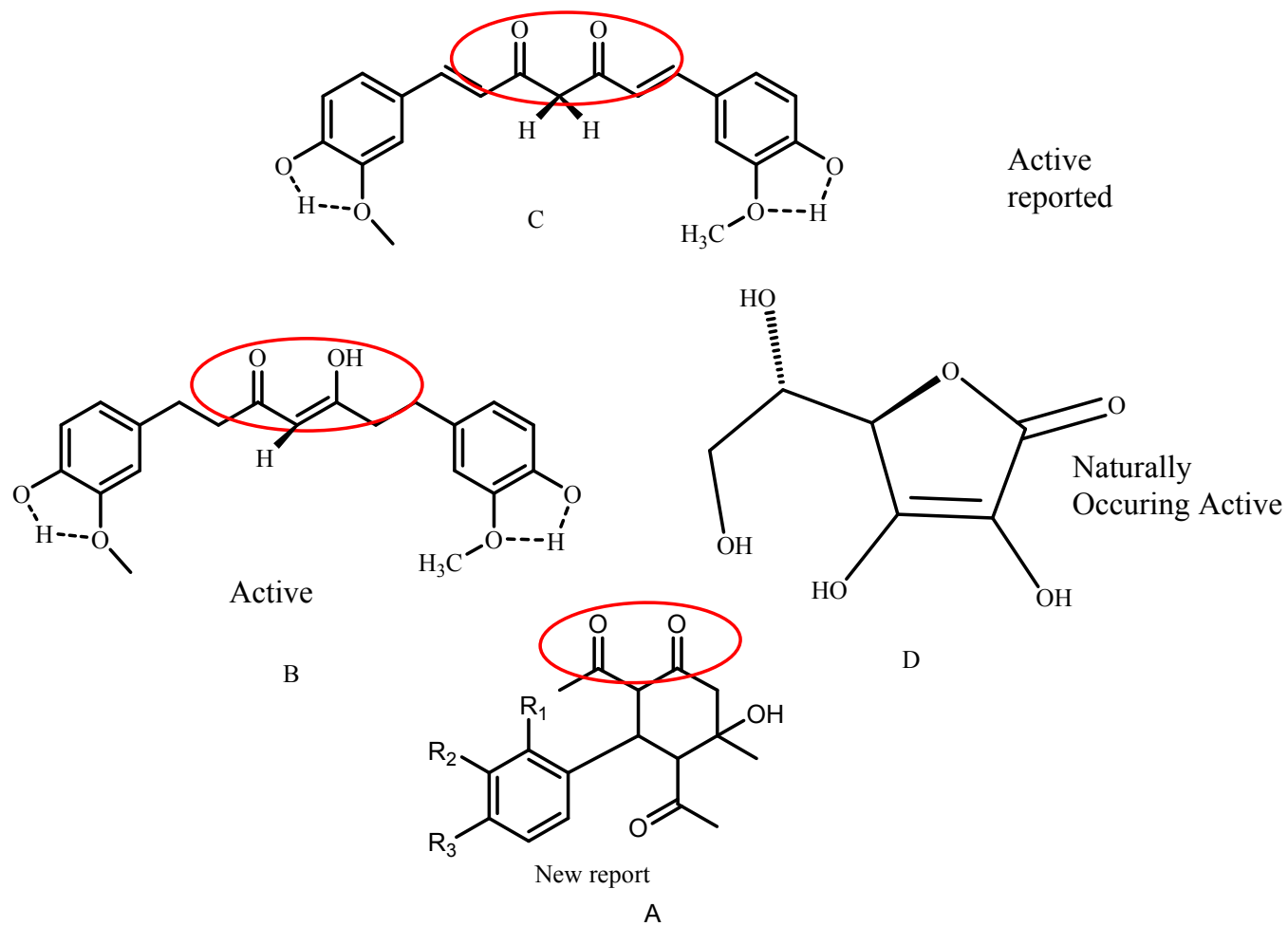
chaired by Dr. Julio A. Seijas Vázquez



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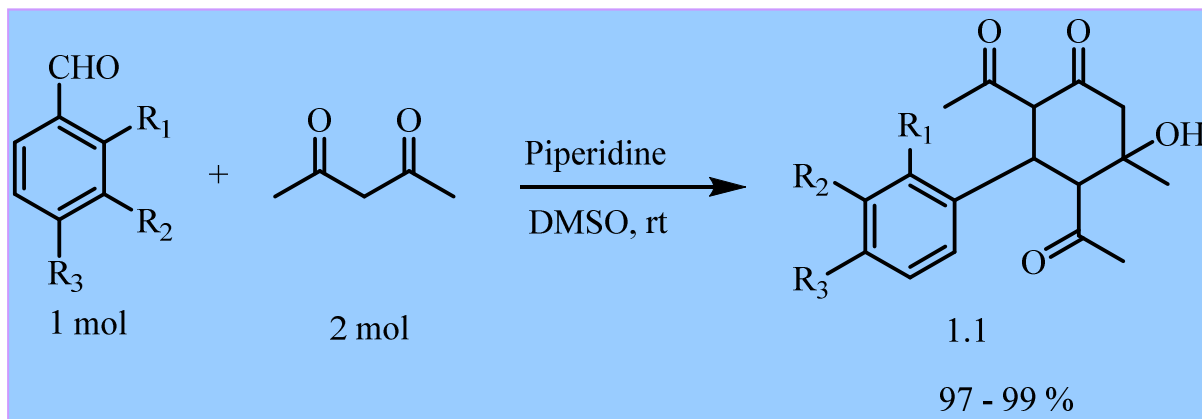
## **SYNTHESIS OF 1, 3 – DIKETOKETONES AS A NOVEL ANTIMICROBIAL, ANTIFUNGAL AND ANTIOXIDANTS AGENTS**

Sunil V. Gaikwad, Avinash M. Patil, Pradeep D. Lokhande\*, Milind D. Nikalje\*



**Cyclohexanone derivatives A having 1,3-diketone moiety B,C,D 1,3diketone have prominent antioxidant activity naturally occurring**

## Scheme1: Synthesis of 2,4-diacetyl-5-hydroxy-5-methyl-3-phenylcyclohexanone derivatives.



1)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{H}$ , 2)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{Cl}$ , 3)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{Br}$ , 4)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{OMe}$ , 5)  $R_1 = \text{NO}_2$   $R_2 = \text{H}$   $R_3 = \text{H}$ , 6)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{NO}_2$ , 7)  $R_1 = \text{F}$   $R_2 = \text{H}$   $R_3 = \text{H}$ , 8)  $R_1 = \text{Cl}$   $R_2 = \text{Cl}$   $R_3 = \text{H}$ , 9)  $R_1 = \text{Br}$   $R_2 = \text{H}$   $R_3 = \text{H}$ , 10)  $R_1 = \text{H}$   $R_2 = \text{NO}_2$   $R_3 = \text{H}$ . 11)  $R_1 = \text{H}$   $R_2 = \text{OMe}$   $R_3 = \text{OMe}$ , 12)  $R_1 = \text{H}$   $R_2 = \text{H}$   $R_3 = \text{CH}_3$

Acetyl acetone 6.07 ml (59.0 mmol), aldehyde 3.0 ml (29.5 mmol) in DMSO 5.0 ml, piperidine 0.583 ml (5.9 mmol) was added, and the reaction mixture was magnetically stirred at ambient temperature. The stirring continued for 5 h the progress of the reaction checked by TLC, after completion of the reaction, the reaction mixture acidified with dil. HCl, quenched into ice cold water, washed with water to afford the pure solid product. Yield: 87 %).

# Antimicrobial Evaluation

An evaluation of the antibacterial activity was done using two Gram-positive, *Bacillus subtilis* (NCIM 2079), *Staphylococcus aureus* (NCIM 2063), and one Gram negative *Escherichia coli* (NCIM 2931) and antifungal *Candida albicans* (NCIM 2091) species, which were collected by Indian Drugs Research Association, Pune (India) from National Chemical Laboratory (NCL) Pune and was assessed for the synthesized cyclohexanone derivatives compounds by well diffusion method.

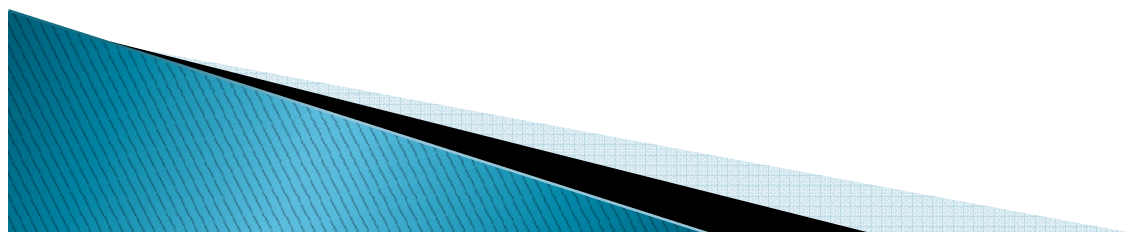
**Table N01. Antimicrobial activity and their MIC value.**

Sample No	Antimicrobial activity			Antifungal
Organism	<i>B. subtilis</i>	<i>S. aureus</i>	<i>E.Coli</i>	<i>C albicans</i>
1	250 PPM	500 PPM	125 ppm	NA
2	250PPM	500PPM	250 ppm	ACTIVE
3	125 PPM	NA	250ppm	NA
4	125PPM	250PPM	100ppm	NA
Ampicillin	50 PPM	100PPM	100 PPM	100PPM

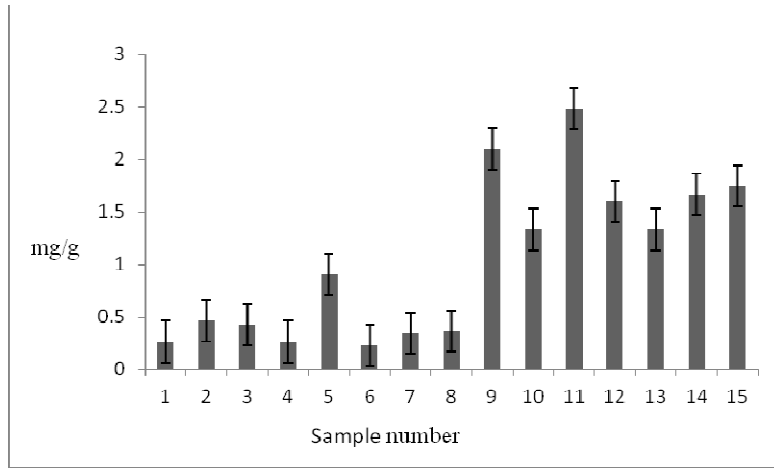
## Antioxidant Activity:

<b>FRAP mg/g Ascorbic acid equivalent</b>	<b>ABTS % Inhibition</b>	<b>DPPH % Inhibition</b>
0.26±0.04	18.64±4.41	14.28±4.65
0.46±0.03	31.63±8.28	27.97±8.72
0.42±0.02	53.38±10.59	50.89±11.16
0.26±0.02	40.39±11.46	37.20±12.08
0.90±0.11	11.58±3.28	6.84±3.46
0.23±0.01	13.84±2.49	9.22±2.62
0.34±0.06	35.59±4.79	32.14±5.05
0.36±0.10	28.81±3.21	48.51±8.84
2.10±0.11	60.45±4.98	58.33±5.25
1.33±0.14	42.65±7.38	16.66±9.42
2.48±0.30	66.94±7.85	57.14±4.07
1.60±0.20	57.06±8.14	49.40±6.93

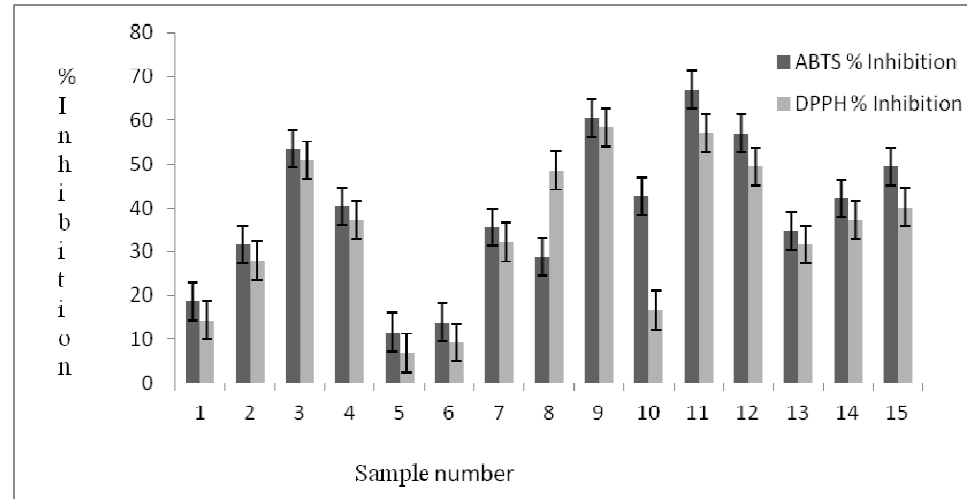
**Table no. 2** Antioxidant activities (FRAP, ABTS and DPPH) of organic compounds. The given values are in triplicates



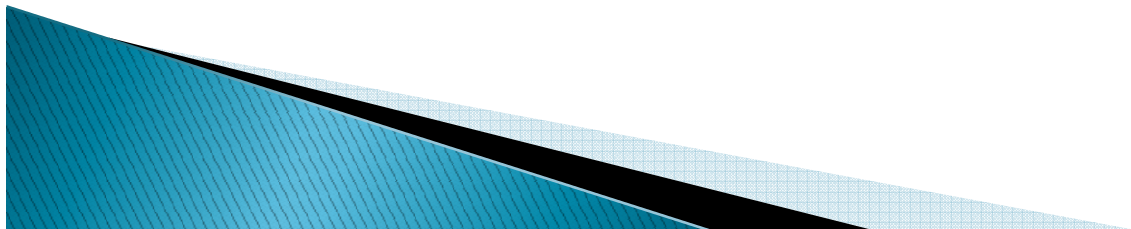
# Antioxidant Activity:



**Figure No. 1** Total antioxidant activity of organic compounds by using FRAPS ferric reducing activity. The values taken are in triplicate basis.



**Figure No. 2** ABTS and DPPH of radical scavenging activity of organic samples. The given values are in triplicates



## X-ray Data Collection, Structure Solution, and Refinement

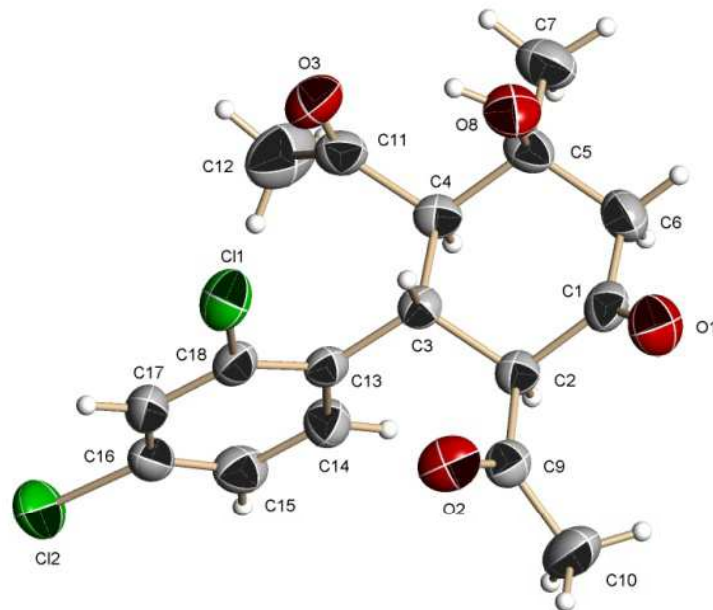


Figure 1. Molecular structure of 4-diacetyl-3-(2,3-dichlorophenyl)-5-hydroxy-5-methylcyclohexanone. Displacement ellipsoids are shown at the 50% probability level.

Full crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. **CCDC-658606**. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: (þ44)1223-336-033; e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)]

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## Sponsors

