Synthesis, spectral correlation and antimicrobial activities of some substituted styryl 5-methyl-2-furyl ketones

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ABSTRACT

A series containing fourteen substituted styryl 5-methyl-2-furyl ketones [2*E*- 1(5-methyl-2-furyl)-3-(substituted phenyl)-2-propen-1-ones] were synthesized by Crossed-Aldol condensation between 2-acetyl-5-methylfuron and various substituted benzaldehydes. The synthesized ketones were characterized by their physical constants and spectral data. The group frequencies of infrared absorption (cm^{-1}) of νCO*s-cis* and *s-trans*, νCH*out of plane* and *in-plane*, νCH=CH *out of plane*, ν>C=C<*out of plane*, ^{1}H chemical shifts (ppm) δH$_\alpha$, δH$_\beta$, ^{13}C chemical shifts (ppm) of δCO, δC$_\alpha$ and δC$_\beta$ of ketones were correlated with various Hammett substituent constants, F, R and Swain-Lupton parameters using single and multi-regression analyses. From the results of statistical analysis, the effects of substituents on the functional group frequencies were studied. The Antimicrobial activities of all ketones have been studied using standard methods.

Introduction

The Hammett correlation of spectral data of organic compounds are useful for the prediction of their structure, stereo-chemical and physicochemical properties[1,2]. The quantitative structure- activity relationship and quantitative property relationship of the organic substrates have been studied from the spectral data associated with their molecular equilibration[3]. The vibrational stretches of carbonyl groups gave two molecular conformers in unsaturated ketones such as *s-cis* and *s-trans* isomers. The *s-cis* carbonyl group stretches are higher than those of the *s-trans* carbonyl group. Based on this the structure of molecular equilibration can be predicted in geometrical isomers, keto-enol tautomers in unsaturated carbonyl compounds[4], alkenes, alkynes, styrenes, nitro-styrenes and naphthacyl ketones and their esters[5]. Nuclear magnetic resonance spectroscopy provides the information about the number of protons present in the molecules and their categories either *E*- or *Z* in the above molecules. These categories of protons can be identified in the organic molecules, based on their coupling constants.. If the molecules possess any substituent in the aromatic ring, corresponding absorption frequencies in IR and the chemical shift in NMR vary from ketone to ketone depending upon the type of substituents whether they are electron donating or electron withdrawing in nature. From these data the effect of substituents can be studied on the particular functional group of the molecule by means of regression analyses[6]. Further these data are employed for the study of transition state reaction mechanism[7], structure activity of biological potentials [8], normal coordinate analysis[9], theoretical study of long range interactions in the beta sheet structures of oligo peptides[10], enone-dienol tautomerism[11], density functional theory[12], rotational barriers in selenomides[13] and gas phase reactivity of alkyl sulphides[14].

The out of plane and in-plane deformation frequencies in fingerprint region are also used for QSAR and QPR study [15]. Generally chalcones possess various multipronged activities [16] such as anticancer, antimicrobial [17], antioxidant [18] antiviral[19], anti-aids [20], insect antifeedant [16], antimalarial [21], anti-plasmodial[22] agrochemicals and drugs[23]. These potentials are also applied for the study of structure activity relationships [24]. From thorough literature survey it is observed that there is no report on the effect of substituents-QSAR or QPR study with these compounds, in the past. Therefore the authors take effort to synthesis some substituted styryl 5-methyl-2-furyl ketones and study the correlation analysis with their IR and NMR data and their antimicrobial activities.

Experimental

General

All chemicals used were purchased from Sigma-Aldrich and E-Merck chemical company. Melting points of all oxiranes have been determined in open glass capillaries on Mettler FP51 melting point apparatus and are uncorrected. Infrared spectra (KBr, 4000-400cm^{-1}) have been recorded on AVATAR-300 Fourier transform spectrophotometer. INSTRUM AV300 NMR spectrometer operating at 300MHz has been utilized for recording ^{1}H spectra and 75.46MHz for ^{13}C spectra in CDCl$_3$ solvent using TMS as internal standard. Electron impact (EI) (70 eV) and chemical ionization mode FAB$^+$ mass spectra have been recorded with a JEOL JMS600H spectrometer.

### Synthesis of substituted styryl 5-methyl-2-furyl ketones

An appropriate equimolar quantity of 2-acetyl-5-methyl-furon (0.01mol), various substituted benzaldehydes (0.01mol), 0.5g of sodium hydroxide and 20 ml of ethanol were warmed in a 50 ml corning conical flask and shaken occasionally[25].The obtained solid was filtered at the pump, washed with cold water

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and crystallized from ethanol afford the respective chalcones as glittering pale yellow solid. The synthesized chalcones are characterized by their physical constants, IR, ^{1}H and ^{13}C NMR and Mass spectral data. Analytical and Mass spectral data are presented in Table-1. Infrared spectral data are given in Table-2. The ^{1}H chemical shifts(ppm) $\delta H\alpha$, $\delta H\beta$, ^{13}C chemical shifts(ppm) of δCO, $\delta C\alpha$ and $\delta C\beta$ of ketones are presented in Table-3.

Results and Discussion
Infrared spectral study

The synthesized chalcones exist as *s-cis* and *s-trans* conformers. These conformers are confirmed by the carbonyl group doublets obtained in the range of 1600-1700cm^{-1}. They are shown in Figure-1 and the corresponding carbonyl frequencies (cm^{-1}) of the conformers are presented in Table-2. The *s-cis* conformers absorb at higher vibrational frequencies than *s-trans* conformers.
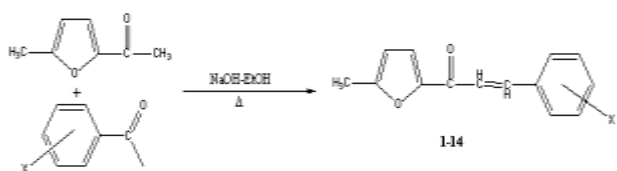
Where X= H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2-NO₂, 3-NO₂, 4-NO₂
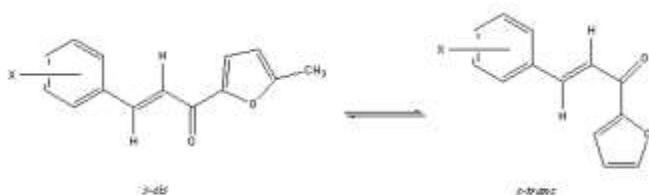
Scheme 1

Figure 1

Generally carbonyl doublets obtained at lower absorption frequencies for the electron donating substituents in the chalcones whereas the electron withdrawing substituents absorb their doublets at higher frequencies in both the conformers. In this present study also, the same trend was observed. These frequencies are correlated with various Hammett sigma constants and Swain-Lupton's parameters[29]by single and multi linear regression analysis. While seeking Hammett correlation involving group frequencies, the form of the Hammett equation employed is

$$\nu = \rho\sigma + \nu_o \qquad ...(1)$$

whereν_o is the frequency for the parent member of the series.

The results of single parameter statistical analysis of carbonyl frequencies with substituent constants are presented in Table-4.The *s-cis*and*s-trans* carbonyl frequencies are correlated satisfactorily with Hammett σ and σ^+ constantsexcept for 4-OH, 2-OCH₃ and 2-NO₂ substituents. All correlations produce positive ρ values. This shows that the normal substituent effects operate in all the conformers. The inductive and resonance effects of the substituents fail in correlations. This is due to the inability to transmit the substituent effect on carbonyl group. Also the inductive effect of the substituents dies off considerably. This is illustrated in the resonance-conjugative structure shown in Figure 2. The substituent effects get reduced, since the substituents are away from three or more carbon bond lengths and this leads to poor correlation. The ratio of $\rho_{s\text{-}cis}$and $\rho_{s\text{-}trans}$ is 1.03.From thisthe ability of transmission of substituent effect on carbonyl group is higher in *s-cis* conformers than in *s-trans* conformers.

The assigned *in-plane* and *out of plane* deformation modes of CH$_{ip}$, CH$_{op}$, CH=CH$_{op}$ and C=C$_{op}$ (cm^{-1})of 5-methyl-2-furyl ketones are presented in Table-2. The larger value of deformation mode frequency for the system is due to the low mobility of electron between the >C = C< and the -CH= CH- frame work. All the deformation modes of substituted styryl 5-methyl-2-furyl ketones are correlated with different substituent constants according to Thirunaraynanet al., [1,3,4-6, 22,24, 25]and John shorter [30]. The results of statistical analysis are shown in Table-4.

The correlation of –CH *in-plane*and *out of plane*deformation stretches with Hammett σ and σ^+seems to be satisfactory excluding halogen and nitro substituents. The correlations with σ_I,σ_R, Fand R parameters are quite bad. This is due to the fact that these parametersare not capable of predicting the substituent effects on CH *in-plane*and *out of plane* modes. All correlations produce positive ρ values. This shows that normal substituent operates in all systems. The failure in correlations is due to the absence of inductive and resonance effects of substituents and it is evidenced by the resonance conjugative structure shownin Figure-2.
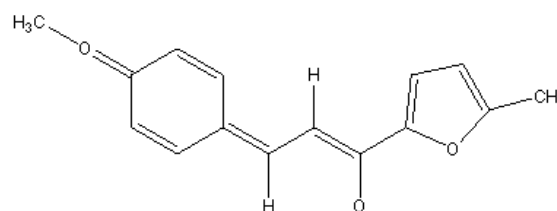

Figure 2

The observed CH=CH *out of plane* frequencies in the present study are given in Table-2. All the deformationCH=CH op modes of stretching frequencies of substituted styryl 5-methyl-2-furyl ketones are correlated with different substituent constants [1,3,4-6, 22,24, 25, 30]. The results of statistical analysis are shown in Table-4. From the Table-4, the r values seem better in Hammett σ, σ^+ and $\sigma_I$constants and they produce the positive ρ values. The other regressions fail in this mode of frequencies with Hammett substituent constants and F and R parameters and they produce negative ρ values. This evidences the operation of reversal of substituent effects on this modes of all ketones.

The observed >C = C< op frequencies in the present study are given in Table-2. All the frequencies of deformation modes of substituted styryl 5-methyl-2-furyl ketones are correlated with different substituent constants[1,3,4-6, 22,24, 25, 30]. The results of statistical analysis are shown in Table-4. The correlation of >C = C< *out of plane* deformation modes with Hammett σ and σ^+seems to be satisfactory. All correlations gave positive ρ values. The correlation with σ_I, σ_R and R values are quite bad. This is due to the fact that these values are not capable of predicting the substituent effects on >C = C< *out of plane* vibrations and the resonance effect of substituents completely absent. This is shown in the conjugative structure inFigure 2 in which the pi-bond character is converted into sigma character.

Some of the single parameter correlations fail with the infrared CO$_{s\text{-}cis}$, CH$_{ip}$, CH$_{op}$, CH=CH$_{op}$ and C=C$_{op}$ with Hammett sigma constants and F and R parameters. While seeking the

multi-regression analysis, satisfactorily correlations are obtained for these stretches with Swain-Lupton and F and R parameters[29]. The correlated multi regression equations are given in 2-13.

$\nu CO_{s\text{-}cis}^{(cm\text{-}1)}$ = 1653.25($\pm$4.315) + 3.742($\pm$0.825)σ_I + 18.318($\pm$0.781) σ_R ...(2)
(R = 0.926, n = 14, P > 90%)

$\nu CO_{s\text{-}cis}^{(cm\text{-}1)}$ = 1651.52($\pm$4.500) + 6.661($\pm$0.854)F +13.024($\pm$0.725)R   ...(3)
(R = 0.953, n = 14, P > 95%)

$\nu CO_{s\text{-}trans}^{(cm\text{-}1)}$ =1599.35($\pm$1.823) − 2.406($\pm$0.348)σ_I − 0.556($\pm$0.033) σ_R ...(4)
(R = 0.923, n = 14, P > 90%)

$\nu CO_{s\text{-}trans}^{(cm\text{-}1)}$ = 1599.74($\pm$1.766) +1.852($\pm$0.335)F +1.322($\pm$0.284)R   ...(5)
(R = 0.922, n = 14, P > 90%)

$\nu\text{-CH}op$ (cm^{-1}) =1152.88($\pm$22.138)-1.058($\pm$0.431) σ_1 - 2.350($\pm$0.547)σ_R ...(6)
(R = 0.901, P>90%, n=14)

$\nu\text{-CH}op$ (cm^{-1}) =1149.208($\pm$21.115) + 8.011($\pm$4.213)F- 2.055($\pm$0.137)R   ...(7)
(R = 0.906, P>90%, n=14)

$\nu\text{-CH}ip$ (cm^{-1}) =1047.64($\pm$6.706) + 36.626($\pm$3.374) σ_1 +0.225($\pm$1.737σ_R ...(8)
(R = 0.917, P>90%, n=14)

$\nu\text{-CH}ip$ (cm^{-1}) =1050.59($\pm$6.837) + 32.173($\pm$13.629)F+ 8.097($\pm$1.378)R   ...(9)
(R = 0.956, P>95%, n=14)

$\nu\text{-CH=CH}op$ (cm^{-1}) = 756.84($\pm$21.223)-17.168($\pm$4.217) σ_1 - 2.334($\pm$0.443)σ_R ...(10)
(R = 0.914, P>90%, n=14)

$\nu\text{-CH = CH-}op$ (cm^{-1}) = 759.75($\pm$20.073) -23.706 ($\pm$4.001)F − 1.834($\pm$0.404 R   ...(11)
(R = 0.902, P>90%, n=14)

$\nu\text{>C = C<}op$ (cm^{-1}) = 548.997($\pm$15.243)+38.470($\pm$3.110) σ_1 +25.733($\pm$3.133)σ_R ...(12)
(R = 0.948, P>90%, n=14)

$\nu\text{>C = C<}op$ (cm^{-1}) = 553.590 ($\pm$14.726)+ 30.912($\pm$2.936) F +33.768($\pm$2.913) R   ...(13)
(R = 0.903, P>90%, n=13)

[1]H Spectral study

The ^{1}H NMR spectra of fourteen chalcones under investigation are recorded in deuterated dimethyl sulphoxide employing tetramethylsilane (TMS) as internal standard. The signals of the ethylenic protons were assigned. They are calculated as AB or AA' BB' systems respectively [1, 31, 32]. The chemical shifts of H_α are at higher field than those of H_β in this series of ketones. The ethylenic protons give an AB pattern and the β-proton doublet in most cases is well separated from the signals of the aromatic protons. The assigned chemical shifts of the ethylenic protons are presented inTable-3.

In nuclear magnetic resonance spectra, the proton chemical shifts δ(ppm) depends on the electronic environment of the nuclei concerned. These shifts can be correlated with reactivity parameters. Thus the Hammett equation may be used in the form as

Log δ= Log δ_0 + ρσ   ... (14)

where$\delta_0$is the chemical shift in the corresponding parent compound.

The assigned ^{1}H NMR chemical shifts (ppm) of $\delta H_\alpha$and δH_β of substituted styryl 5-methyl-2-furyl ketones are presented in Table-3. These chemical shifts are correlated with Hammett

substituent constants and F and R parameters. The results of statistical analysis these chemical shifts (ppm) are shown in Table-5. From the Table-5, Hammett σ, σ$^+$ and σ_R constants correlated satisfactorily with H_α chemical shifts except for 3-Br, 3-OCH$_3$ and 3-NO$_2$ substituents. All correlations gave positive ρ values. This shows that the normal substituent effects operate in all ketones. The polar, inductive, field and resonance effects failed in correlation. This is due to the incapability of substituents for predicting the reactivity through the substituent effects on the vinyl H_α proton chemical shifts which is associated with the conjugative structure in Figure 2.The H_β chemical shifts of these ketones failed in correlation with Hammett sigma constants and F and R parameters. During the correlation, all Hammett constants and F and R parameters gave negative ρ values. This shows that the normal substituent effects are reversed in all ketones.

Some of the single parameter correlations fails with the ^{1}H NMR of δH_α and δH_βchemical shifts with Hammett sigma constants and F and R parameters. While seeking the multi regression analysis of these frequencies, there is satisfactorily correlations obtained with Swain-Lupton and F and R parameters. The correlated multi regression equations are, (15-18)

δH_α(ppm) = 7.370($\pm$0.138) +0.226($\pm$0.026)σ_I + 0.441($\pm$0.025) σ_R ...(15)
(R = 0.956, n = 14, P > 950%)

δH_α (ppm) = 7.402($\pm$0.123) +0.194($\pm$0.042)F +0.458($\pm$0.021)R   ...(16)
(R = 0.960, n = 14, P > 95%)

δH_β(ppm) =7.654($\pm$0.150) +0.178($\pm$0.027)σ_I - 0.271($\pm$0.027)σ_R ...(17)
(R = 0.923, n = 14, P > 90%)

δH_β(ppm) = 7.691($\pm$0.148) + 0.103($\pm$0.028)F -0.184($\pm$0.023)R   ...(18)
(R = 0.937, n = 14, P > 90%)

^{13}C NMR spectral study

The assigned carbonyl carbon chemical shifts (ppm) of δCO, δC_α and $\delta C_\beta$of substituted styryl-5-methyl-2-furyl ketones are presented in Table-3 and these chemical shifts are correlated with Hammett sigma constants and F and R parameters. The results of statistical analysis is shown in Table-5.From the Table-5,it is evident that the chemical shifts (ppm) of CO carbon, correlated satisfactorily with the Hammett σ_I and σ_R constants, except for H, 4-F, 2-OCH$_3$ and 4-CH$_3$ substituents. All correlations gave positive ρ values. This means that the normal substituent effects operate in all ketones. Hammett σ and σ$^+$ constants and field effects failed in correaltion. This is due to the reason stated earlier which is associated with the conjugtive structurein Figure-2.
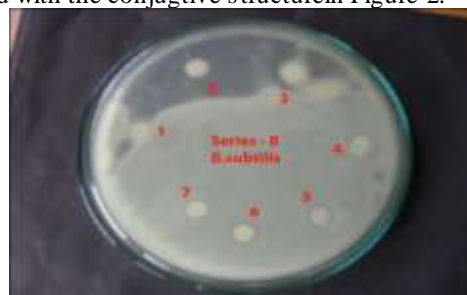
Plate-1

Plate-2

Plate-3

Plate-4

Plate-5

Plate-6

Plate-7

Plate-8

Plate-9

Plate-10

Plate-11
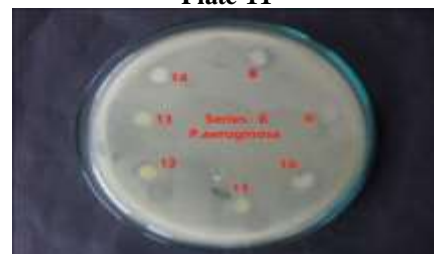
Plate-12

Figure 3. Antibacterial activities of substituted styryl 5-methyl-2-furyl ketones (Plates 1-12).

The assigned chemical shifts (ppm) of C_α and C_β vinyl carbons in the substituted styryl 5-methyl-2-furyl ketones were correlated with Hammett sigma constants and F and R parameters. The C_α chemical shifts correlated satisfactorily with Hammett σ, σ^+ constants, and F and R parameters except for 4-F, 4-CH₃ and 4-NO₂ substituents. All correlations gave positive ρ values. This shows that the normal substituent effects operate in all ketones.The inductive effects of the substituents failed in correlation. This is due to the reason stated earlier as per the conjugated structure given in Figure-2.

The C_β chemical shifts (ppm) in substituted styryl 5-methyl-2-furyl ketones produced satisfactory correlation with Hammett sigma constants and F and R parameters except for 3-Br, 4-F, 2-OCH₃,3-NO₂and 4-NO₂ substituents. All correlations gave negative ρ values, while resonance effects of the substituents gave positive ρ values. Inductive effects of the substituents failed in correlation. This is due to the reason stated earlier and is associated with the conjugated structure in Figure-2.

Single parameter correlations fails with the ^{13}C NMR of δC_α and δC_β chemical shifts(ppm) with Hammett sigma constants and F and R parameters. While seeking the multi-regression analysis of these frequencies, there is satisfactorily correlations obtained with Swain-Lupton and F and R parameters. The correlated multi regression equations are in19-24.

$$\delta CO(ppm) = 177.71(\pm2.343) +3.294(\pm0.448)\sigma_I + 7.902(\pm2.135)\sigma_R \quad ...(19)$$
$(R = 0.956, n = 14, P > 95\%)$

$$\delta CO (ppm) = 178.12(\pm2.204) +2.959(\pm0.418)F +7.929(\pm2.267)R \quad ...(20)$$
$(R = 0.960, n = 14, P > 95\%)$

$$\delta C_\alpha(ppm) =121.82 (\pm1.335) + 1.907(\pm0.259)\sigma_I + 0.941(\pm0.024)\sigma_R \quad ...(21)$$
$(R = 0.928, n = 14, P > 90\%)$

$$\delta C_\alpha(ppm) =122.182 (\pm1.328) + 1.214(\pm0.252)F +1.225(\pm0.214)R \quad ...(22)$$
$(R = 0.924, n = 14, P > 90\%)$

$$\delta C_\beta(ppm) =143.05 (\pm2.208) -4.645(\pm0.422)\sigma_I + 3.755(\pm0.402)\sigma_R \quad ...(23)$$
$(R = 0.935, n = 14, P > 90\%)$

$$\delta C_\beta(ppm) =142.73 (\pm2.164) -3.785(\pm0.411)F +2.988(\pm0.349) R \quad ...(24)$$
$(R = 0.932, n = 14, P > 90\%)$

Microbial activities

Chalcones possess a wide range of biological activities such as antibacterial [17], antifungal[17], antiviral [19], antifeedant[16], anticancer[17], antimalarial[21], antituberculosis[33], antiAIDS[20] and antioxidant[18] activities. These multipronged activities present in different chalcones are examined against respective microbes-bacteria's, and fungi.

Collection of Microorganisms

Bacillus subtilis, Escherichia coli, Klebsila pneumonia, Micrococcus luteus, Pseudomonas aerogenosa, Staphylococcus areus, Aspergillusniger, Mucor species and*Trichodermaviride* were procured from the Research department of Microbiology, Sengunthar Arts and Science College, Thiruchengode, Namakkal Dt., Tamilnadu.

Innoculum preparation

The nutrient broth was procured from Himedia, Mumbai. The nutrient broth was prepared by weighing 1.3gram, of the broth and dissolved it in 100 ml of sterile distilled water. The flask was swirled gently while adding the nutrient broth and the

pH of the medium was adjusted to 7.0. The Erleumayer flask was plugged with non-adsorbent cotton and sterilized in an autoclave at 121°C and 15lbs/inc² pressure for 15 minutes. After cooling inside a laminar flow, a loopful of fresh bacterial sample was inoculated and incubated in an orbital shaker at 37°C for 24 hours. Then the cultures were diluted 1:50 with sterile physiological saline and 0.5 ml of the innoculum was used for the preparation of the spread plate. The same procedure has been adopted for all test bacterial samples.

Preparation of agar slants

Nutrients agar medium was prepared and sterilized in an autoclave at 121°C and 15 lbs/inc² pressure for 15 minutes. After sterilization the medium was dispensed into the test tubes. The test tubes were kept in the slanting position on a support. After complete solidification of the medium, streaking of the microorganism was done in the slant area using sterile inoculation loop. After the streaking the test tubes were incubated at 37°C for 24 hours. After good growth, the slants have been stored in a deep freezer (2°C) for further studies.

Preparation of Mueller Hinton agar plates

The Mueller Hinton agar of weight 38 gram was dissolved in 1000 ml of sterile distilled water. The pH of the medium was adjusted to 7.0. The flask was plugged with cotton and sterilized at 121°C and 15 lbs/inc² pressure for 15 minutes. After sterilization, the medium was cooled to 45-47o C, poured 15 ml of it in each sterile Petri-plates and allowed to solidify.

Preparation of test compound

The newly synthesized Chalcone compounds of weight 15 mg of each was dissolved in 1 ml of DMSO solvent. Using 100 µml solution, the discs were impregnated and placed on the Mueller Hinton solidified Agar medium to find out the antimicrobial activity of the compounds on each organism. By adapting the above procedure, the antimicrobial activity of the five series of chalcones has been studied on six microorganisms and the results have been discussed.

Antibacterial sensitivity assay

Antibacterial sensitivity assay was performed using Kirby-Bauer[34] disc diffusion technique. In each Petri plate about 0.5 ml of the test bacterial sample was spread uniformly over the solidified Mueller Hinton agar using sterile glass spreader. Then the discs with 5mm diameter made up of Whatman No.1 filter paper, impregnated with the solution of the compound were placed on the medium using sterile forceps. The plates were incubated for 24 hours at 37°C by keeping the plates upside down to prevent the collection of water droplets over the medium.

After 24 hours, the plates were visually examined and the diameter values of the zone of inhibition were measured. Triplicate results were recorded by repeating the same procedure.

The antibacterial screening effect of synthesized chalcones is shown in Figure-3. (Plates 1-12). The zone of inhibition is compared using Table-6 and the Clustered column Chart is shown in Figure-4. A very good antibacterial activity was possessed by all substituents on the microorganisms in general. All the compounds showed excellent activities on *E.coli*and*P.aeruginosa* species. The –CH₃ substituent has improved antibacterial activity against *M.luteus*. The nitro substituent has satisfactory effect on all microorganisms.
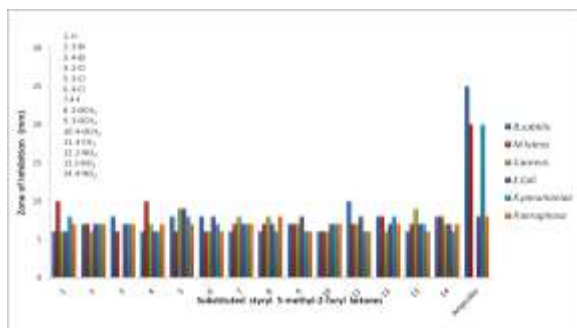
Figure 4. Antibacterial activities of substituted styryl 5-methyl-2-furyl ketones-zone of inhibition chart

Antifungal activity

Preparation of the Potato dextrose agar medium

PDA agar medium was prepared in a conical flask by dissolving 3.9gram of the agar in 100ml distilled water. It was sterilized in the autoclave for 15min. at 121°C and 15 lbs/inch^2 pressure. Then the medium was allowed for solidification for an hour. After that the fungal species was inoculated in the medium and kept for 5 to 7 days at room temperature.

Preparation of the fungal innoculam

About 20 to 25 ml of sterile water (after cooling) was mixed with the medium. The water over the medium was swirled and decanted with the fungal species. Tweeen-80(1 to 2 ml) have been added with this solution for uniform growth.

Antifungal sensitivity assay

Antifungal sensitivity assay was performed using Kirby-Bauer[34]disc diffusion technique. PDA medium was prepared and sterilized as above. It was poured (ear bearing heating condition) in the Petri-plate which was already filled with 1 ml of the fungal species. The plate was rotated clockwise and counter clock-wise for uniform spreading of the species. The discs were impregnated with the test solution. The test solution was prepared by dissolving 15mg of the Chalcone in 1ml of DMSO solvent. The medium was allowed to solidify and kept for 24 hours. Then the plates were visually examined and the diameter values of zone of inhibition were measured. Triplicate results were recorded by repeating the same procedure.

The antifungal activity of substituted chalcones synthesized in the present study are shown in Figure-5 for Plates (1-6) and the zone of inhibition values of the effect is given in Table-7. The clustered column chart, shown in Figure-6 reveals that all the compounds have excellent antifungal activity against all the three fungal species namely *A.niger,M.spp*and*T.viride.* The Chalcones with 3-Br, 3-Cl, 4-F, 2-OCH$_3$ and 4-CH$_3$ substituents have shown greater antifungal activity than those with the other substituents present in the series.
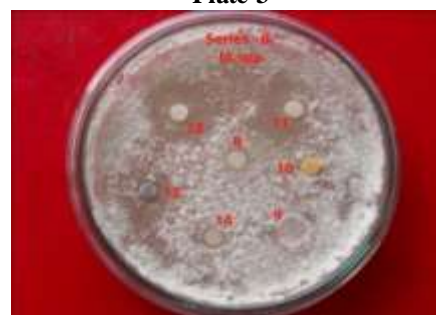

Plate-2

Plate-3

Plate-4

Plate-5

Plate-1

Plate-6

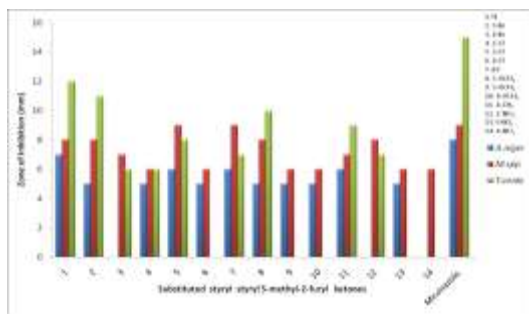**Figure-5.Antifungal activities of substituted styryl 5-methyl-2-furyl ketones (plates 1-6)**

Figure-6. Antifungal activities of substituted styryl 5-methyl-2-furyl ketones-zone of inhibition chart

Acknowledgement

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Table-1 Analytical, physical constants and Mass data of substituted styryl 5-methyl-2-furyl ketones

Entry	Substituent	Molecular Formulae	Molecular Weight	M.p.(℃)	Mass(m/z)
1	H	$C_{14}H_{12}O_2$	212	111-112 (110)[26]	212[M+]
2	3-Br	$C_{14}H_{11}BrO_2$	195	112-113	195[M+], 197[M+2]
3	4-Br	$C_{14}H_{11}BrO_2$	195	159-160	207[M+], 209[M+2]
4	2-Cl	$C_{14}H_{11}ClO_2$	236	139-140	236[M+], 238[M+2]
5	3-Cl	$C_{14}H_{11}Cl O_2$	236	71-72 (73)[27]	236[M+], 238[M+2]
6	4-Cl	$C_{14}H_{11}Cl O_2$	236	145-146	236[M+], 238[M+2]
7	4-F	$C_{14}H_{11}F O_2$	239	88-89	239[M+], 242[M+2]
8	2-OCH$_3$	$C_{15}H_{14}O_3$	242	74-75	242[M+]
9	3- OCH$_3$	$C_{15}H_{14}O_3$	242	122-123	242[M+]
10	4- OCH$_3$	$C_{15}H_{14}O_3$	242	116-117	242[M+]
11	4- CH$_3$	$C_{15}H_{14} O_2$	226	108-09	226[M+]
12	2-NO$_2$	$C_{14}H_{11}NO_4$	257	118-119	257[M+]
13	3- NO$_2$	$C_{14}H_{11}NO_4$	257	122-123 (122)[28]	257[M+]
14	4- NO$_2$	$C_{14}H_{11}N O_4$	257	133-134	257[M+]

Table-2 Infrared spectral data v(cm⁻¹) of CO*s-cis*and *s-trans*stretches,CH*ip* and *op*, CH=Ch*op* and>C=C<*op* modes of substituted styryl-5-methyl-2-furyl ketones

Entry	Substituent	CO*s-cis*	CO*s-trans*	CH*op*	CH*ip*	CH=CH*op*	>C=C<*op*
1	H	1652.64	1600.98	1143.23	1063.81	775.84	570.33
2	3-Br	1655.38	1600.90	1172.13	1068.61	782.46	579.73
3	4-Br	1651.02	1601.38	1172.65	1064.94	774.13	541.98
4	2-Cl	1654.26	1601.40	1128.69	1053.78	756.65	585.20
5	3-Cl	1653.28	1601.34	1101.73	1066.88	792.22	582.81
6	4-Cl	1651.32	1594.70	1107.32	1063.76	733.21	541.88
7	4-F	1650.98	1599.28	1157.38	1065.11	735.99	547.11
8	2-OCH$_3$	1647.00	1601.73	1181.21	1065.23	729.13	548.03
9	3-OCH$_3$	1655.26	1602.04	1168.32	1062.58	718.56	542.36
10	4-OCH$_3$	1649.85	1597.30	1159.35	1068.23	716.58	541.98
11	4-CH$_3$	1649.71	1597.43	1171.46	1028.78	727.09	515.53
12	2-NO$_2$	1654.51	1603.83	1173.38	1072.77	705.42	562.85
13	3-NO$_2$	1658.20	1597.91	1172.60	1070.44	742.44	581.23
14	4-NO$_2$	1655.53	1602.75	1178.54	1078.21	743.58	582.19

Table-3 The ¹H chemical shifts(ppm)of δHα, δHβ, ¹³C chemical shifts of δCO, δCα, δCβ and ring carbons of substituted styryl 5-methyl-2-furyl ketones

Entry	Substit.	δHα (1H, *d*)	δHβ (1H, *d*)	Ring protons	Substt.	δCO	δCα	δCβ	Substt.
1	H	7.658	7.807	7.662-7.793 (7H, *m*)	---	179.05	122.66	144.94	---
2	3-Br	7.760	7.380	7.654-7.377 (6H, *m*)	---	176.74	123.00	136.98	---
3	4-Br	7.780	7.380	7.753-7.365 (6H, *m*)	---	183.25	124.62	140.71	---
4	2-Cl	7.410	8.290	7.421-7.798 (6H, *m*)	---	176.78	123.92	138.85	---
5	3-Cl	7.377	7.767	7.385-7.354 (6H, *m*)	---	176.70	122.49	141.44	---
6	4-Cl	7.300	7.790	7.371-7.865 (6H, *m*)	---	176.87	121.69	141.68	---
7	4-F	7.317	7.812	7.325-7.764 (6H, *m*)	---	176.97	121.08	141.85	---
8	2-OCH$_3$	7.267	7.818	7.283-7.780 (6H, *m*)	2.341 (3H, *s*)	178.71	121.01	142.83	57.96 (3H, *s*)
9	3-OCH$_3$	6.855	7.817	7.012-7.763 (6H, *m*)	2.255 (3H, *s*)	171.00	123.57	137.01	59.26 (3H, *s*)
10	4-OCH$_3$	7.271	7.822	7.278-7.779 (6H, *m*)	2.273 (3H, *s*)	171.09	121.25	136.74	55.32 (3H, *s*)
11	4-CH$_3$	7.347	7.836	7.438-7.799 (6H, *m*)	2.221 (3H, *s*)	177.17	120.01	143.12	27.76 (3H, *s*)
12	2-NO$_2$	7.482	7.838	7.498-7.773 (6H, *m*)	---	179.05	122.66	144.94	---
13	3-NO$_2$	7.820	7.883	7.723-7.802 (6H, *m*)	---	176.74	123.00	136.98	---
14	4-NO$_2$	7.304	7.502	7.321-7.498 (6H, *m*)	---	183.25	124.62	140.71	---

Table-4 Results of statistical analysis of infrared ν (cm^{-1}) CO$_{s\text{-}cis}$ and CO$_{s\text{-}trans}$, CHip and op, CH=CHop and >C=C<op modes of substituted styryl5-methyl-2-furyl ketones with Hammett σ, σ^+, σ_I, σ_R constants and F and R parameters

Frequency	Constants	r	I	ρ	s	n	Correlated derivatives
CO$_{s\text{-}cis}$	σ	0.966	1648.44	13.240	5.76	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ^+	0.963	1649.33	9.891	5.98	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ_I	0.828	1647.54	9.583	7.40	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	σ_R	0.861	1654.93	19.458	6.11	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	F	0.821	1647.43	9.500	7.40	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2-NO₂,3-NO₂, 4-NO₂
	R	0.850	1654.48	14.072	6.69	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4-NO₂
CO$_{s\text{-}trans}$	σ	0.932	1599.72	2.215	2.48	11	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ^+	0.947	1599.69	2.51	2.31	11	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_I	0.822	1599.18	2.583	2.56	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_R	0.811	1600.44	1.249	2.61	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	F	0.819	1599.33	2.414	2.58	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	R	0.816	1600.57	1.614	5.95	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃,4-CH₃, 2- NO₂,3-NO₂, 4-NO₂

Table continued

Frequency	Constants	r	I	ρ	s	n	Correlated derivatives
CHop	σ	0.904	1157.55	-3.911	0.97	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ^+	0.914	154.74	-9.346	0.96	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ_I	0.805	1153.38	-1.263	1.40	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	σ_R	0.819	1152.44	-2.448	1.11	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	F	0.678	1149.57	8.090	3.40	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	R	0.804	1158.23	-2.382	1.69	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4-NO₂
CHip	σ	0.905	1058.15	18.199	1.48	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ^+	0.900	1059.02	15.961	1.31	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_I	0.851	1047.56	36.641	2.29	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_R	0.820	1062.84	13.631	2.76	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	F	0.808	1049.15	31.680	2.99	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	R	0.817	1063.51	8.806	2.02	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂

Table continued

Frequency	Constants	r	I	ρ	s	n	Correlated derivatives
CH=CHop	σ	0.900	750.32	0.395	1.72	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ^+	0.911	748.83	7.950	1.96	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F,2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4NO₂
	σ_I	0.901	757.34	-17.369	1.40	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	σ_R	0.603	749.70	-3.931	5.15	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	F	0.820	760.08	-21.632	3.23	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2-NO₂,3-NO₂, 4-NO₂
	R	0.800	750.24	-0.885	3.91	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃,2- NO₂,3-NO₂, 4-NO₂
>C=C<op	σ	0.905	552.03	34.511	1.90	11	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ^+	0.907	551.54	41.021	1.69	11	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_I	0.814	543.46	40.679	2.51	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	σ_R	0.887	564.99	29.303	2.67	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	F	0.801	547.58	29.607	2.48	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂
	R	0.817	565.99	35.527	2.13	14	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH₃, 3-OCH₃, 4-OCH₃, 4-CH₃, 2- NO₂,3-NO₂, 4-NO₂

r = Correlation co-efficient; ρ = Slope; I = Intercept; s = Standard deviation; n = Number of substituents

Table-5 Results of statistical analysis of ^{1}H chemical shifts(ppm)of δHα, δHβ protons, ^{13}C chemical shifts of δCO, δCα and δCβ carbons of of substituted styryl5-methyl-2-furyl ketones with Hammett σ, σ$^+$, σ$_I$,σ$_R$ constants and F and R parameters

Chemical shifts	Constants	r	ρ	I	s	n	Correlated derivatives
δ$_{Hα}$(ppm)	σ	0.944	0.270	7.319	0.21	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$, 4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 4-NO$_2$
	σ$^+$	0.928	0.135	7.351	0.22	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 4-NO$_2$
	σ$_I$	0.805	0.366	7.233	0.22	14	H, 3-Br,4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$,3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	σ$_R$	0.952	0.500	7.472	0.20	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 4-NO$_2$
	F	0.820	0.294	7.285	0.22	14	H, 3-Br,4-Br,2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$,3-OCH$_3$,4-OCH$_3$,4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	R	0.957	0.488	7.488	0.15	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 4-NO$_2$
δ$_{Hβ}$(ppm)	σ	0.805	-0.521	7.780	2.22	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	σ$^+$	0.809	0.092	7.738	0.22	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	σ$_I$	0.824	-0.219	7.734	0.21	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	σ$_R$	0.806	0.065	7.749	0.26	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	F	0.827	-0.168	7.737	0.21	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$
	R	0.817	-0.178	7.621	0.23	14	H, 3-Br, 4-Br, 2-Cl,3-Cl,4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$,3-NO$_2$,4-NO$_2$

Table continued

Chemical shifts	Constants	r	ρ	I	s	n	Correlated derivatives
δCO(ppm)	σ	0.839	4.089	176.66	3.66	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	σ$^+$	0.839	3.136	176.92	3.67	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	σ$_I$	0.933	5.808	175.25	3.76	11	3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 3-NO$_2$, 4-NO$_2$
	σ$_R$	0.953	8.580	179.19	3.36	12	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	F	0.827	4.690	175.64	3.84	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	R	0.857	8.365	179.43	3.26	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
δCα(ppm)	σ	0.932	1.631	122.04	1.87	13	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$
	σ$^+$	0.945	1.791	122.03	1.70	13	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$
	σ$_I$	0.925	2.206	121.52	1.97	12	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$
	σ$_R$	0.918	1.492	122.68	1.97	12	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 2-NO$_2$, 3-NO$_2$
	F	0.917	1.482	121.80	1.95	12	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 2-NO$_2$, 3-NO$_2$
	R	0.919	1.416	122.72	1.94	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$

Table continued

Chemical shifts	Constants	r	ρ	I	s	n	Correlated derivatives
δCβ(ppm)	σ	0.914	-1.240	140.79	3.28	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2NO$_2$
	σ$^+$	0.912	-0.861	140.69	3.29	11	H, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2NO$_2$
	σ$_I$	0.821	-3.452	141.89	3.22	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	σ$_R$	0.917	2.411	140.97	3.26	11	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-Cl, 4-F, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 3NO$_2$
	F	0.922	-3.133	141.80	3.23	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F,2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$
	R	0.919	2.392	141.05	3.25	14	H, 3-Br, 4-Br, 2-Cl,3-Cl, 4-Cl, 4-F, 2-OCH$_3$, 3-OCH$_3$,4-OCH$_3$, 4-CH$_3$, 2-NO$_2$, 3-NO$_2$, 4-NO$_2$

r = Correlation co-efficient; ρ = Slope; I = Intercept; s = Standard deviation; n = Number of substituents

Table-6 Antibacterial activity of substituted styryl 5-methyl-2-furyl ketones

Entry	Compound	R	Zone of Inhibition (mm)					
			Gram positive Bacteria			Gram negative Bacteria		
			B.subtilis	*M.luteus*	*S.aureus*	*E.coli*	*K.pneumoniae*	*P.aeruginosa*
1	B-1	H	6	10	6	6	8	7
2	B-2	3-Br	7	7	6	7	7	7
3	B-3	4-Br	8	6	-	7	7	7
4	B-4	2-Cl	6	10	7	6	6	7
5	B-5	3-Cl	8	6	9	9	8	7
6	B-6	4-Cl	8	6	6	8	7	6
7	B-7	4-F	6	7	8	7	7	7
8	B-8	2-OCH$_3$	6	7	8	7	6	8
9	B-9	3-OCH$_3$	7	7	7	8	6	6
10	B-10	4-OCH$_3$	6	6	6	7	7	7
11	B-11	4-CH$_3$	10	7	7	8	6	6
12	B-12	2-NO$_2$	8	8	6	7	8	7
13	B-13	3-NO$_2$	6	7	9	7	7	6
14	B-14	4-NO$_2$	8	8	7	7	6	7
	Standard	Ampicillin	25	20	-	8	20	8
	Control	DMSO	-	-	-	-	-	-

Table-7 Antifungal activities of substituted styryl 5-methyl-2-furyl ketones

Entry	Compound	R	Zone of Inhibition (mm		
			A.niger	*M.spp*	*T.viride*
1	B-1	H	7	8	12
2	B-2	3-Br	5	8	11
3	B-3	4-Br	-	7	6
4	B-4	2-Cl	5	6	6
5	B-5	3-Cl	6	9	8
6	B-6	4-Cl	5	6	-
7	B-7	4-F	6	9	7
8	B-8	2-OCH$_3$	5	8	10
9	B-9	3-OCH$_3$	5	6	-
10	B-10	4-OCH$_3$	5	6	-
11	B-11	4-CH$_3$	6	7	9
12	B-12	2-NO$_2$	-	8	7
13	B-13	3-NO$_2$	5	6	-
14	B-14	4-NO2	-	6	-
	Standard	Miconazole.	8	9	15