



## Synthesis, spectral, electrochemical and antimicrobial studies of some 2-pyrrolyl chalcones

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### ABSTRACT

A series containing twelve substituted styryl 2-pyrrolyl ketones have been synthesized by solvent free fly-ash:H<sub>2</sub>SO<sub>4</sub> solid acid catalysed crossed aldol condensation. These chalcones were characterized by their physical constants and spectral data. The IR and NMR spectral frequencies of  $\nu_{CO}$ -*cis* and *s-trans*, deformation modes of  $\nu_{CHip}$ , *op*, CH=CH*op* and C=C*op*(cm<sup>-1</sup>),  $\delta H$  and  $\delta C$  of  $\alpha$ ,  $\beta$  and CO(ppm) and the electrochemical reduction potential and currents of carbonyl and vinyl groups of synthesized chalcones were correlated with Hammett substituent constants, F and R parameters. From the results of statistical analyses the effects of substituents on the group frequencies and electrochemical functionalities have been discussed. The antimicrobial activities of all chalcones have been studied using Bauer-Kirby method.

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### Introduction

The Quantitative structure activity relationship and quantitative structure property relationships were used for finding the structure of molecule, quantitative and qualitative analysis[1]. Spectral data are useful for prediction of ground state equilibration of organic molecules such as *s-cis* and *s-trans* isomers of alkenes, alkynes, benzoylchlorides, styrenes and  $\alpha$ ,  $\beta$ -unsaturated ketones[2]. Their use in structure parameter correlations becomes popular for studying biological activities[3], normal co-ordinate analysis[4] and transition states of reaction mechanisms[5]. Infrared spectroscopy is a powerful technique for the qualitative and quantitative study of natural and synthetic molecules[2]. IR spectroscopy can provide information about the nature, concentration and structure of samples at the molecular level[7]. A great deal of work has been devoted to the reactivity of  $\alpha$ , $\beta$ -carbonyl compounds particularly, the theoretical study of substituent effects has been studied on long range interactions in the  $\beta$ -sheet structure[8] of oligo-peptides, enone-dienol tautomerism[9]. 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[10]. 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 maximum absorption in UV, 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 analysis [11]. Now a day's scientists [12] have paid more interest to correlate the group frequencies of spectral data with Hammett substituent constants to explain the substituent effects of organic compounds. Recently Thirunarayanan et al

[13], investigated elaborately the single and multi-substituent effects on alpha and beta hydrogen and carbons of furyl chalcones. Redox potentials of organic molecules are very useful for studying electrochemical behaviour such as oxidation, reduction and group transformation process. These processes are essential for conversion of one functional group into another by electron transfer. Electrochemical synthesis is another kind process for the study of properties of reactant and products[14]. Boykin and co-workers [15] have studied the dc polarographic redox potential of chalcones and they found to good correlation with sigma constants. Alston and Fry[16] investigates the reduction potential correlation with Hammett sigma *para*-constants for the chalcone system having substituents in both phenyl rings. These system performs for evaluation of Bekkum, Verkade and Wepster correlation with correlation parameters. Moraleda et. al. [17] have studied to found good correlation of  $\alpha$ , $\beta$ -unsaturated carbonyl compounds with half-wave potential, LUMO-HOMO energies with Hammett  $\sigma p$  constants. There is no report available for the correlation of redox potential and current of C=C and CO of substituted styryl 2-pyrrolyl ketones with Hammett substituent constants, F and R parameters in literature in the past. Hence the authors have taken efforts to study the electrochemical behaviour of 2-pyrrolyl chalcones through the correlation of redox potential with Hammett substituent constants, Field and Resonance parameters. Chalcones (1, 3-diaryl-2-propen-1-ones) constitute an important class of natural products belonging to the flavonoids family, display interesting biological activities including anticancer, anti-inflammatory, antioxidant, cytotoxic, antimicrobial, analgesic and antipyretic, anti-anginal, anti-hepatotoxic, antimalarial, anti-allergic and antifeedant. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three carbon  $\alpha$ , $\beta$ -unsaturated Carbonyl system[1-3]. From the chemical studies on the

structure of clavacin, it was found that the structural feature, responsible for the antibacterial activity was  $\alpha$ ,  $\beta$ -unsaturated keto functional group[4]. The diverse properties of chalcones have prompted us to synthesize them and study their antimicrobial activity. However there is no information available regarding the study of UV, IR, NMR spectral, electrochemical and microbial study in literature in the past for substituted styryl-2-pyrrolyl ketones. Hence the authors have taken efforts to synthesize some substituted styryl-2-pyrrolyl ketones by solvent free fly:ash-H<sub>2</sub>SO<sub>4</sub> solid acid catalyzed crossed aldol condensation of 2-acetylpyrrole with various *o*-, *m*- and *p*-substituted benzaldehydes and to study the quantitative structure property relationships as well as their antimicrobial activities.

## Experimental

### Materials and methods

All chemicals were procured from E-Merck brand. Fly ash was collected from Thermal Power Plant-II, Neyveli Lignite Corporation (NLC), Neyveli, Tamil Nadu, India. Melting points of all chalcones were determined in open glass capillaries on Mettler FP51 melting point apparatus and are uncorrected. Infrared spectra (KBr, 4000-400 cm<sup>-1</sup>) were recorded on an Avatar-300 Fourier transform spectrophotometer. The NMR spectra of unknown compounds were recorded in Bruker AVIII 5000 spectrometer operating at 500 MHz for <sup>1</sup>H NMR spectra and 125.46 MHz for <sup>13</sup>C NMR spectra in CDCl<sub>3</sub> solvent using TMS as internal standard. Electron impact (EI, 70 eV) and chemical ionization mode FAB<sup>+</sup> mass spectra were recorded with a Varian 500 spectrometer.

### Preparation and characterization of catalyst

In a 50 mL Borosil beaker, 1g of Fly-ash and 0.8 mL (0.5 mol) of sulphuric acid were taken and mixed thoroughly with glass rod. This mixture was heated on a hot air oven at 85° C for 1 h, cooled to room temperature, stored in a Borosil bottle and tightly capped. This was characterized by infrared spectra. Infrared spectral data of Fly-ash: H<sub>2</sub>SO<sub>4</sub> is  $\nu$  (cm<sup>-1</sup>): 3456 (OH); 3010 (C-H); 1495, 1390(C-S); 1336, 1154 (S=O); and *out of plane* modes: 1136, 1090, 976, 890, 850, 820, 667, 658, 620, 580, 498, 425.

### Synthesis of substituted styryl 2-pyrrolyl ketones

An appropriate equi-molar quantities of pyrrole-2-methyl ketones (2 mmol), substituted benzaldehydes (2 mmol) and Fly-ash: H<sub>2</sub>SO<sub>4</sub>(0.5 g) were taken in Borosil tube and tightly capped. The mixture was subjected to microwave heated for 5-6 minutes in a microwave oven (Scheme 1) (LG Grill, Intellowave, Microwave Oven, 160-800W) and then cooled to room temperature. The organic layer was separated with dichloromethane and the solid product was obtained on evaporation. The solid, on recrystallization with benzene-hexane mixture gave glittering pale yellow solid. The insoluble catalyst was recycled by washing the solid reagent remained on the filter by ethyl acetate (8 mL) followed by drying in an oven at 100°C for 1h and it was made reusable for further reactions.

### Voltammetry

The Reduction potential of these chalcones was determined in HCH Instruments inc., Electrochemical Analyzer USA using platinum wire electrode in spectral grade methanol.

## Results and Discussion

### Ultra violet spectral study

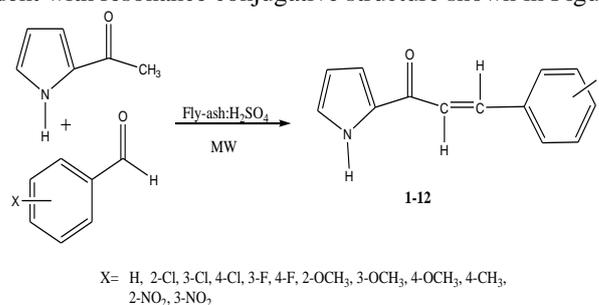
The UV spectra of all synthesized chalcones were recorded in SHIMADZU-1650 SPECTROMETER ( $\lambda_{\max}$  nm) in spectral grade methanol. The measured absorption maxima ( $\lambda_{\max}$  nm) of these chalcones are presented in Table 2. These values are

correlated with Hammett substituent constants and F and R parameters using single and multi-linear regression analysis[10]. Hammett correlation involving the group frequencies and absorption maxima, the form of the Hammett equation employed is

$$\lambda = \rho\sigma + \lambda_0 \quad \dots(1)$$

where  $\lambda_0$  is the frequency for the parent member of the series.

The results of statistical analysis[1,2,11-13] of these values with Hammett substituent constants are presented in Table 3. From Table 3, Hammett substituent constants  $\sigma$ ,  $\sigma^+$ ,  $\sigma_R$ ,  $\sigma_I$  and R values gave poor correlations with  $\lambda_{\max}$ . All constants gave positive  $\rho$  values except  $\sigma_I$  constants. This is due to the inductive effects of the substituents were weak for predicting the reactivity on the absorption through resonance. This is evident with resonance conjugative structure shown in Figure 1.



Scheme 1

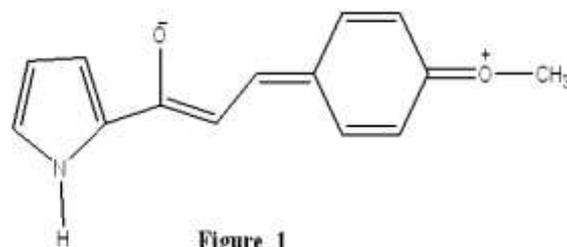


Figure 1

The multi regression analysis of these frequencies of all ketones with inductive, resonance and Swain – Lupton's [18] constants produce satisfactory correlations as evident in equations 2 and 3.

$$\lambda_{(nm)} = 342.24(\pm 4.858) + 1.175(\pm 0.962)\sigma_I - 3.949(\pm 0.822)\sigma_R \quad \dots(2)$$

$$(R = 0.914, n = 12, P > 90\%)$$

$$\lambda_{(nm)} = 343.655(\pm 4.509) - 2.035(\pm 0.855)F - 2.823(\pm 0.771)R \quad \dots(3)$$

$$(R = 0.913, n = 12, P > 90\%)$$

### 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<sup>-1</sup>. They are shown in Figure-2 and the corresponding carbonyl frequencies (cm<sup>-1</sup>) of the conformers are presented in Table-2. The *s-cis* conformers absorbs at higher vibrational frequencies than *s-trans* conformers. 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 [18] by single and multi linear regression analysis[1,2,10-13, ]. While seeking Hammett correlation involving group frequencies, the form of the Hammett equation employed is

$$\nu = \rho\sigma + \nu_0 \quad \dots(4)$$

where  $\nu_0$  is the frequency for the parent member of the series.

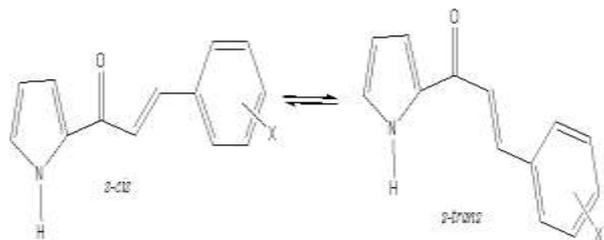


Figure 2

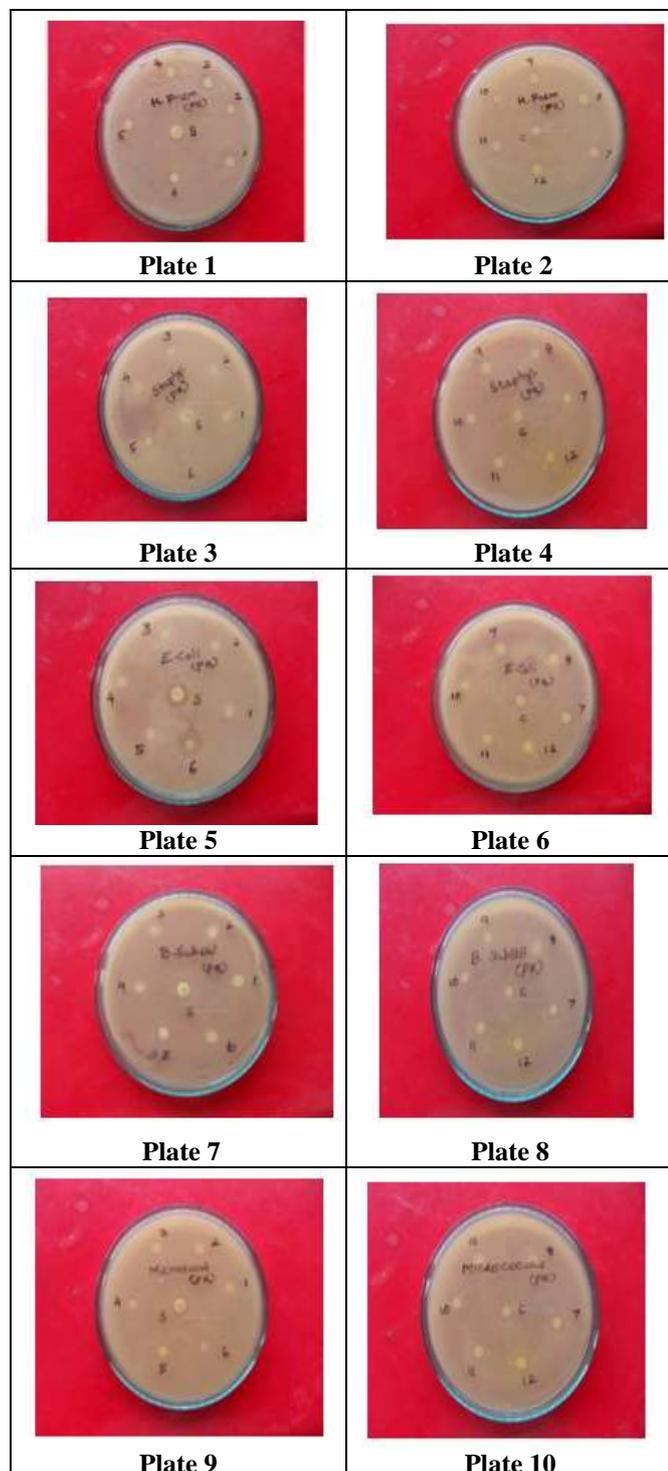


Fig 3. Antibacterial activity of styryl 2-pyrrolyl ketones

The results of single parameter statistical analysis of carbonyl frequencies with substituent constants are presented in Table-3. From Table 3, the *s-cis* and *s-trans* conformers the correlation  $\nu_{C=O}$  of both conformers fails with Hammett  $\sigma$  constants and F and R parameters. Both conformers correlated satisfactorily with Hammett sigma values and other values were fail. All correlations gave positive  $\rho$  values and it implies that there is a normal substituent effects operates in all systems. This failure in correlation is due the conjugation between the substituent and the carbonyl group in chalcones as shown in Figure 1.

The correlation of CH *in-plane* and *out of plane* modes with Hammett sigma constants were fails in correlation. The CH *in-plane* modes gave negative  $\rho$  values in all correlation and it implies that the substituent effects were reverses. On the other hand the CH *out of plane* modes gave positive  $\rho$  values and this reveals that there is a normal substituent effects operated in all ketones. The failure in correlation was due to the reason stated earlier and associated with the resonance conjugative structure shown in Fig. 1.

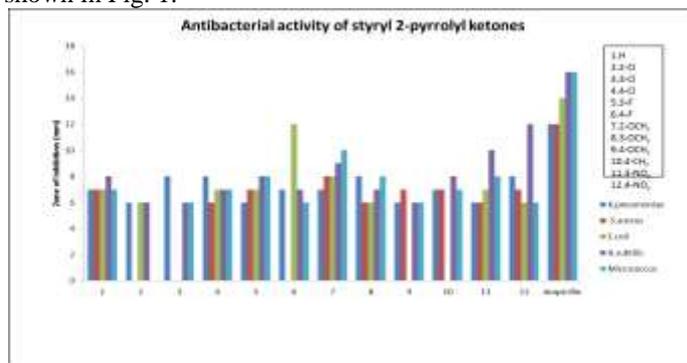


Fig. 4 Antibacterial activity of styryl 2-pyrrolyl ketones: Clustered column chart

All correlation were fails with CH=CH *out of plane* modes with Hammett constants, F and R parameters. On the other hand C=C *out of plane* modes with Hammett  $\sigma_R$  constants correlated satisfactorily. All correlation gave positive  $\rho$  values and this reveals that there is a normal substituent effects operated in all ketones. In the correlation of C=C *out of plane modes* with the remaining sigma constants and R parameter gave negative  $\rho$  values and it implies that there is a reversal of substituent effects operated in these system. This is due to the reason stated earlier and associated with the resonance conjugative structure shown in Fig. 1.

In view of the inability of some of the  $\sigma$  constants to produce individually satisfactory correlations, it was thought that worthwhile to seek multiple correlations involving either  $\sigma_1$  and  $\sigma_R$  constants or Swain-Lupton's [11], F and R parameters. The correlation equations for *s-cis*, *s-trans* and *deformation modes* are given in equations 5-16.

$$\nu_{CO_{s-cis}}^{(cm^{-1})} = 1646.04(\pm 1.815) + 3.351(\pm 0.359) \sigma_1 + 3.594(\pm 0.330) \sigma_R \quad \dots(5)$$

$$(R = 0.945, n = 12, P > 90\%)$$

$$\nu_{CO_{s-cis}}^{(cm^{-1})} = 1646.13(\pm 1.668) + 3.348(\pm 0.316)F + 3.683(\pm 0.278)R \quad \dots(6)$$

$$(R = 0.942, n = 12, P > 90\%)$$

$$\nu_{CO_{s-trans}}^{(cm^{-1})} = 1577.25(\pm 13.851) + 50.906(\pm 27.444)\sigma_1 - 17.000(\pm 2.518)\sigma_R \quad \dots(7)$$

$$(R = 0.953, n = 12, P > 95\%)$$

$$\nu_{CO_{s-trans}}^{(cm^{-1})} = 1578.12(\pm 12.189) + 50.968(\pm 23.147)F - 4.467(\pm 2.108)R \quad \dots(8)$$

( $R = 0.959$ ,  $n = 12$ ,  $P > 95\%$ )

$$\nu\text{CH}_{ip}^{(\text{cm}^{-1})} = 1120.12(\pm 12.152) - 11.750(\pm 2.401) \sigma_I - 48.428(\pm 2.281) \sigma_R \quad \dots(9)$$

( $R = 0.961$ ,  $n = 12$ ,  $P > 95\%$ )

$$\nu\text{CH}_{ip}^{(\text{cm}^{-1})} = 1117.10(\pm 10.455) - 10.228(\pm 19.851)F - 49.799(\pm 1.801)R \quad \dots(10)$$

( $R = 0.967$ ,  $n = 12$ ,  $P > 95\%$ )

$$\nu\text{CH}_{op}^{(\text{cm}^{-1})} = 846.142(\pm 10.441) + 22.196(\pm 2.269) \sigma_I - 2.361(\pm 0.187) \sigma_R \quad \dots(11)$$

( $R = 0.933$ ,  $n = 12$ ,  $P > 90\%$ )

$$\nu\text{CH}_{op}^{(\text{cm}^{-1})} = 846.60(\pm 9.431) + 23.117(\pm 17.921)F + 3.822(\pm 1.673)R \quad \dots(12)$$

( $R = 0.939$ ,  $n = 12$ ,  $P > 90\%$ )

$$\nu\text{CH}=\text{CH}_{op}^{(\text{cm}^{-1})} = 1054.57(\pm 12.881) + 16.372(\pm 2.558) \sigma_I + 10.000(\pm 2.314) \sigma_R \quad \dots(13)$$

( $R = 0.926$ ,  $n = 12$ ,  $P > 90\%$ )

$$\nu\text{CH}=\text{CH}_{op}^{(\text{cm}^{-1})} = 1058.97(\pm 12.110) + 6.986(\pm 2.229)F + 12.115(\pm 2.094)R \quad \dots(14)$$

( $R = 0.920$ ,  $n = 12$ ,  $P > 90\%$ )

$$\nu\text{C}=\text{C}_{op}^{(\text{cm}^{-1})} = 557.941(\pm 13.431) + 18.798(\pm 2.661) \sigma_I - 34.713(\pm 2.417) \sigma_R \quad \dots(15)$$

( $R = 0.945$ ,  $n = 12$ ,  $P > 90\%$ )

$$\nu\text{C}=\text{C}_{op}^{(\text{cm}^{-1})} = 560.22(\pm 12.750) + 14.012(\pm 2.421)F - 25.157(\pm 2.205)R \quad \dots(16)$$

( $R = 0.940$ ,  $n = 12$ ,  $P > 90\%$ )

#### $^1\text{H}$ NMR spectral study

The  $^1\text{H}$  NMR spectra of synthesized chalcones were recorded in deuteriochloroform solutions employing tetramethylsilane (TMS) as internal standard. The signals of the ethylenic protons were assigned from their spectra. They were calculated as AB or AA' or BB' systems respectively. The lower chemical shifts (ppm) obtained for  $\text{H}_\alpha$  and higher chemical shifts (ppm) obtained for  $\text{H}_\beta$  in this series of ketones. The vinyl protons give an AB pattern and the  $\beta$ -proton doublets were well separated from the signals of the aromatic protons. The assigned vinyl proton chemical shifts  $\delta$ (ppm) of all ketones were presented in Table 4.

In nuclear magnetic resonance spectra, the proton or the  $^{13}\text{C}$  chemical shifts ( $\delta$ ) depends on the electronic environment of the nuclei concerned. The assigned vinyl proton chemical shifts (ppm) have been correlated with reactivity parameters using Hammett equation in the form of

$$\text{Log } \delta = \text{Log } \delta_0 + \rho\sigma \quad \dots (17)$$

Where  $\delta_0$  is the chemical shift of unsubstituted ketones.

The assigned  $\text{H}_\alpha$  and  $\text{H}_\beta$  proton chemical shifts (ppm) are correlated with various Hammett sigma constants. The results of statistical analysis [1,2, 10-13] are presented in Table 5. All correlation were fail for  $\text{H}_\alpha$  and  $\text{H}_\beta$  proton chemical shifts (ppm) with Hammett sigma constants, F and R parameters. The positive  $\rho$  values were obtained in all correlation and are evident for the normal substituent effect operates in all chalcones for  $\text{H}_\alpha$ . The negative  $\rho$  values were obtained in all correlation and are evident for the normal substituent effect was reversed in all chalcones for  $\text{H}_\beta$  proton chemical shifts (ppm). These failure in correlation is due to the reasons stated in earlier and the conjugative structure shown in Figure 1.

Application of Swain-Lupton [18] treatment to the relative chemical shifts of  $\text{H}_\alpha$  and  $\text{H}_\beta$  with F and R values is successful with resonance, inductive and fail with F & R parameter generates the multi regression equations 18-21.

$$\delta\text{H}_\alpha(\text{ppm}) = 7.217(\pm 0.076) + 0.121(\pm 0.015) \sigma_I + 0.100(\pm 0.013) \sigma_R \quad \dots(18)$$

( $R = 0.935$ ,  $n = 12$ ,  $P > 90\%$ )

$$\delta\text{H}_\alpha(\text{ppm}) = 7.202(\pm 0.070) + 0.140(\pm 0.013)F + 0.078(\pm 0.010)R \quad \dots(19)$$

( $R = 0.936$ ,  $n = 12$ ,  $P > 90\%$ )

$$\delta\text{H}_\beta(\text{ppm}) = 7.807(\pm 0.035) - 0.029(\pm 0.003) \sigma_I - 0.088(\pm 0.061) \sigma_R \quad \dots(20)$$

( $R = 0.915$ ,  $n = 12$ ,  $P > 90\%$ )

$$\delta\text{H}_\beta(\text{ppm}) = 7.784(\pm 0.032) + 0.012(\pm 0.006)F + -0.033(\pm 0.005)R \quad \dots(21)$$

( $R = 0.919$ ,  $n = 12$ ,  $P > 90\%$ )

#### $^{13}\text{C}$ NMR spectral study

Spectral analysts, organic chemists and scientists[[1,2, 10-13] have made extensive study of  $^{13}\text{C}$  NMR spectra for a large number of different ketones and styrenes. The assigned vinyl  $\text{C}_\alpha$ ,  $\text{C}_\beta$  and carbonyl carbon chemical shifts are presented in Table 4. The results of statistical analysis are given in Table 5. They have been observed a poor correlation for the chemical shifts(ppm) of  $\text{C}_\alpha$  carbon with Hammett  $\sigma$  constants, F and R parameters. A satisfactory correlation obtained for  $\text{C}_\beta$  carbon with Hammett sigma constants and F parameters with negative  $\rho$  values. The remaining inductive and resonance parameters fails in correlations. This is due to reasons stated earlier with the resonance conjugative structure shown in Figure 1.

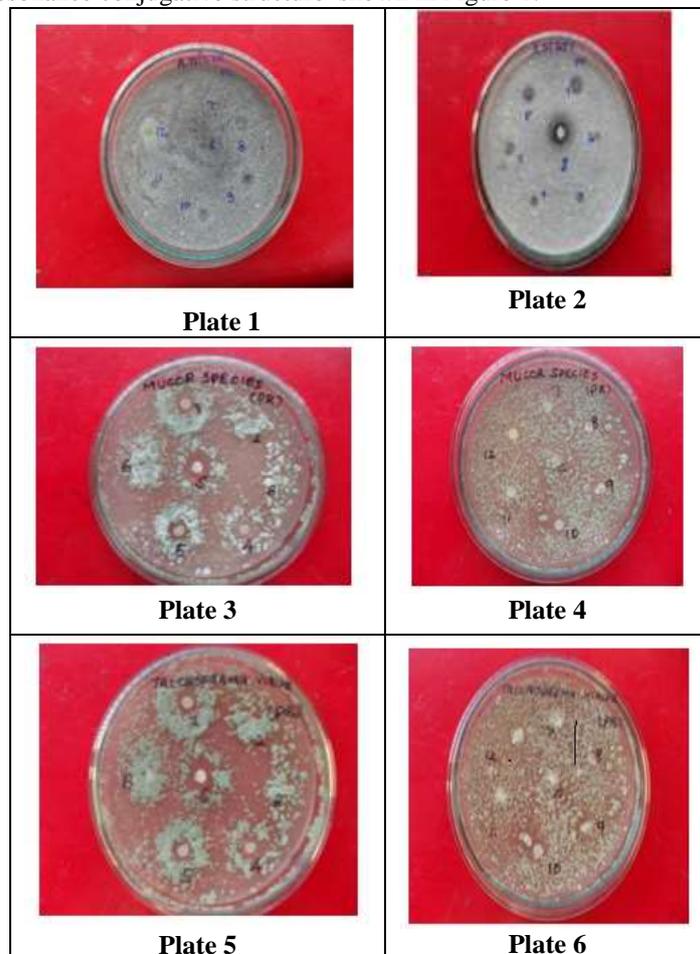


Fig. 5. Antifungal activity of styryl 2-pyrrolyl ketones

The assigned carbonyl carbon chemical shifts (ppm) were correlated with Hammett constants using single and multi linear regression analysis and it presented in Table 5. The Hammett sigma constants only correlated satisfactorily with carbonyl carbon chemical shifts of ketones. All correlations gave negative  $\rho$  values and it is evident for the normal substituent effects was reversed in all ketones. This is due to the

conjugation exists between the substituent and the carbonyl group shown in Figure 1.

The Swain Luptons' [18] parameter correlations were satisfactorily obtained within these carbon chemical shifts and the regression equations are given in 22-27

$$\delta C_{\alpha} (\text{ppm}) = 122.58 (\pm 1.769) + 2.939 (\pm 0.350) \sigma_I - 0.306 (\pm 0.002) \sigma_R \quad \dots(22)$$

$$(R = 0.926, n = 12, P > 90\%)$$

$$\delta C_{\alpha} (\text{ppm}) = 122.67 (\pm 1.619) + 2.943 (\pm 0.237)F + 0.655 (\pm 0.287)R \quad \dots(23)$$

$$(R = 0.930, n = 12, P > 90\%)$$

$$\delta C_{\beta} (\text{ppm}) = 142.17 (\pm 0.233) - 3.380 (\pm 0.047) \sigma_I + 1.463 (\pm 0.043) \sigma_R \quad \dots(24)$$

$$(R = 0.994, n = 12, P > 95\%)$$

$$\delta C_{\beta} (\text{ppm}) = 141.85 (\pm 0.265) - 2.819 (\pm 0.517)F - 1.947 (\pm 0.548)R \quad \dots(25)$$

$$(R = 0.973, n = 12, P > 95\%)$$

$$\delta CO (\text{ppm}) = 1178.70 (\pm 0.314) - 1.292 (\pm 0.062) \sigma_I - 1.289 (\pm 0.005) \sigma_R \quad \dots(26)$$

$$(R = 0.973, n = 12, P > 95\%)$$

$$\delta CO (\text{ppm}) = 178.41 (\pm 0.034) - 0.774 (\pm 0.057)F - 1.466 (\pm 0.052)R \quad \dots(27)$$

$$(R = 0.970, n = 12, P > 95\%)$$

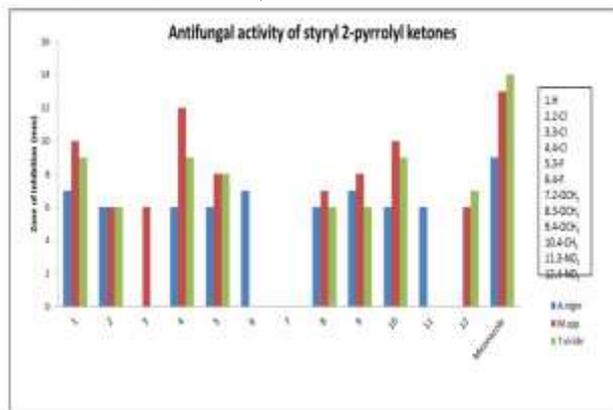


Fig. 6. Substituted styryl 2-pyrrolyl ketones: Clustered column chart

#### Electrochemical study

In the present study the ketones were chosen as an  $\alpha,\beta$ -unsaturated system. These system exhibit as *E*-stable conformers. The measured reduction potential (*v*) and the corresponding current (*i*) are presented in Table 6. These potential and currents are correlated with Hammett substituent constants, *F* and *R* parameters using single and multi-regression analyses[1, 2, 10-13]. The results of statistical analysis of reduction potential (*v*) and the corresponding current (*i*) with Hammett substituent constants, *F* and *R* parameters are presented in Table 7. From Table 7, correlation of reduction potential of *C=C* with sigma constants, *F* and *R* parameters were fail. On the other hand this current (*i*) were satisfactory correlated with sigma constants, *F* and *R* parameters. The  $\sigma_R$  constant is fail with these parameters. This is due to the inability of effect of substituents not obeyed the potential and current and the conjugation between the substituent and carbonyl group shown in Figure 2. All correlation gave negative  $\rho$  values except  $\sigma_R$  with reduction potential of *C=C* and vice versa with *C=C* current. All correlations are fail with the reduction potential of *CO* with sigma constants, *F* and *R* parameters. A satisfactory correlation obtained for *R* parameter with reduction current of *CO*. Remaining sigma constants and Field

parameters fail in correlations. This failure was due to conjugative structure shown in Figure 1.

Some of the single parameter electrochemical correlations were fails with Hammett sigma constants, *F* and *R* parameters. On the other hand the multi-regressions were worthwhile and leads to satisfactory correlation with Swain[18] *F* and *R* parameters collectively. The correlation equations 28-35 are as

$$C=C(v) = 0.486 (\pm 0.211) - 0.290 (\pm 0.065) \sigma_I + 0.129 (\pm 0.048) \sigma_R \quad \dots(28)$$

$$(R = 0.915, n = 14, P > 90\%)$$

$$C=C(v) = 0.430 (\pm 0.020) - 0.422 (\pm 0.046)F - 0.165 (\pm 0.032)R \quad \dots(29)$$

$$(R = 0.927, n = 14, P > 90\%)$$

$$C=C(i) = -3.360 (\pm 1.467) + 9.383 (\pm 3.287) \sigma_I - 3.168 (\pm 0.245) \sigma_R \quad \dots(30)$$

$$(R = 0.968, n = 14, P > 95\%)$$

$$C=C(i) = 1.328 (\pm 0.134) + 0.780 (\pm 0.289)F + 3.115 (\pm 0.211)R \quad \dots(31)$$

$$(R = 0.940, n = 14, P > 90\%)$$

$$C=O(v) = -2.494 (\pm 0.105) + 1.917 (\pm 0.023) \sigma_I - 4.749 (\pm 0.176) \sigma_R \quad \dots(32)$$

$$(R = 0.964, n = 14, P > 95\%)$$

$$C=O(v) = -0.869 (\pm 0.096) + 0.804 (\pm 0.218)F + 1.111 (\pm 0.011)R \quad \dots(33)$$

$$(R = 0.921, n = 14, P > 90\%)$$

$$C=O(i) = -2.632 (\pm 0.313) - 0.323 (\pm 0.069) \sigma_I + 0.668 (\pm 0.058) \sigma_R \quad \dots(34)$$

$$(R = 0.901, n = 14, P > 90\%)$$

$$C=O(i) = -4.962 (\pm 2.038) + 3.399 (\pm 0.461)F - 3.731 (\pm 0.327)R \quad \dots(35)$$

$$(R = 0.942, n = 14, P > 90\%)$$

#### Antimicrobial activities

##### Microbial activities

Chalcones possess a wide range of biological activities such as antibacterial[19], antifungal[19], antiviral[20], antifeedant[21], anticancer[19], antimalarial[22], antituberculosis[23], antiAIDS[24] and antioxidant[25] activities. These multiprolonged activities present in different chalcones are examined against respective microbes-bacteria's and fungi.

##### Antibacterial sensitivity assay

Antibacterial sensitivity assay was performed using Kirby-Bauer[26] 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 Whatmann 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 1-10). The zone of inhibition is compared using Table-8 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 *K.pneumoniae* and *B.subtilis* species. The substituent 2-OCH<sub>3</sub>, 3-NO<sub>2</sub> and 4-NO<sub>2</sub> have high activity against *B.subtilis*. The substituent 4-F

has improved antibacterial activity against *E.Coli* than other species.

#### Antifungal sensitivity assay

Antifungal sensitivity assay was performed using Kirby-Bauer[26] 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 activities 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-9. 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* except 2-OCH<sub>3</sub> substituent. The chalcones with H, 3-Cl, 3-F, 4-OCH<sub>3</sub> and 4-CH<sub>3</sub> substituents have shown greater antifungal activity than those with the other substituents present in the series.

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**Table 1. Physical constants and mass spectral data of substituted styryl 2-pyrrolyl ketones**

Entry	X	Molecular Formula	Molecular Weight	m.p.(°C)	Mass (m/z)
1	H	C <sub>13</sub> H <sub>11</sub> NO	197	135-137	197[M <sup>+</sup> ], 131,120,103,94,77,66
2	2-Cl	C <sub>13</sub> H <sub>10</sub> NOCl	231	122-124	231[M <sup>+</sup> ], 233[M <sup>2+</sup> ], 196,167,139,120,111,94,66,77
4	3-Cl	C <sub>13</sub> H <sub>10</sub> NOCl	231	>360	231[M <sup>+</sup> ], 233[M <sup>2+</sup> ], 196,167,168,139,140,120,111,94,66,77
5	4-Cl	C <sub>13</sub> H <sub>10</sub> NOCl	231	155-157	231[M <sup>+</sup> ], 233[M <sup>2+</sup> ], 196,167,147,139,119,120,111,94,77,66
6	3-F	C <sub>13</sub> H <sub>10</sub> NOF	215	>360	215[M <sup>+</sup> ], 217[M <sup>2+</sup> ], 198,149,121,120,94,77
7	4-F	C <sub>13</sub> H <sub>10</sub> NOF	215	86-88	215[M <sup>+</sup> ], 217[M <sup>2+</sup> ], 198,186,149,121,120,94,77,66
8	2-OCH <sub>3</sub>	C <sub>14</sub> H <sub>13</sub> NO <sub>2</sub>	227	>360	227[M <sup>+</sup> ], 196,163,134,120,106,94,77,66
9	3-OCH <sub>3</sub>	C <sub>14</sub> H <sub>13</sub> NO <sub>2</sub>	227	110-112	227[M <sup>+</sup> ], 212,196,163,154,134,120,106,94,77,66
10	4-OCH <sub>3</sub>	C <sub>14</sub> H <sub>13</sub> NO <sub>2</sub>	227	134-136	227[M <sup>+</sup> ], 198,196,156,163,134,119,103,94,77,66
11	4-CH <sub>3</sub>	C <sub>14</sub> H <sub>13</sub> NO	211	148-150	211[M <sup>+</sup> ], 196,145,119,115,94,91,77,66
12	3-NO <sub>2</sub>	C <sub>13</sub> H <sub>11</sub> NO <sub>3</sub>	243	128-130	242[M <sup>+</sup> ], 178,176,148,121,120,94,77
12	4-NO <sub>2</sub>	C <sub>13</sub> H <sub>11</sub> NO <sub>3</sub>	243	201-203	242[M <sup>+</sup> ], 195,178,176,167,148,121,120,102,94,77

Table 2. UV and IR spectral data of substituted styryl 2-pyrrolyl ketones

Entry	X	UV $\lambda_{\max}(\text{nm})$	IR $\nu(\text{cm}^{-1})$						Substt.
			CO <i>s-cis</i>	CO <i>s-trans</i>	CH <sub>ip</sub>	CH <sub>op</sub>	CH=CH <sub>op</sub>	C=C <sub>op</sub>	
1	H	338.0	1649.0	1591.2	1110.0	839.7	1045.3	570.9	---
2	2-Cl	341.2	1647.1	1627.8	1116.7	866.5	1068.5	563.2	---
3	3-Cl	339.0	1647.1	1593.1	1112.9	866.2	1056.9	580.5	---
4	4-Cl	342.0	1647.1	1624.1	1112.9	867.9	1086.2	561.2	---
5	3-F	341.2	1647.1	1627.8	1112.9	866.8	1018.3	563.2	---
6	4-F	337.0	1647.1	1635.5	1162.0	872.2	1086.2	603.7	---
7	2-OCH <sub>3</sub>	354.5	1643.4	1579.2	1136.2	846.4	1049.4	598.2	1234.5
8	3-OCH <sub>3</sub>	340.5	1645.2	1585.4	1134.1	844.8	1051.1	596.2	1258.1
9	4-OCH <sub>3</sub>	354.5	1645.2	1569.9	1170.7	823.5	1058.8	557.4	1236.8
10	4-CH <sub>3</sub>	342.5	1643.2	1583.4	1132.1	866.1	1056.9	545.8	---
11	3-NO <sub>2</sub>	339.0	1652.9	1598.9	1114.8	858.3	1058.8	592.1	---
12	4-NO <sub>2</sub>	354.0	1643.2	1589.2	1109.0	844.8	1064.6	545.8	---

Table 3. Results of statistical analysis of UV  $\lambda_{\max}(\text{nm})$ , infrared  $\nu(\text{cm}^{-1})$  of CO *s-cis* and CO *s-trans*, CH<sub>ip</sub> and *op*, CH=CH<sub>op</sub> and >C=C<sub>op</sub> modes of substituted styryl 2-pyrrolyl ketones with Hammett  $\sigma$ ,  $\sigma^+$ ,  $\sigma_I$ ,  $\sigma_R$  constants and F and R parameters.

Functionality	Const.	r	I	$\rho$	s	n	Correlated derivatives
$\lambda_{\max}$	$\sigma$	0.624	344.35	-4.434	6.77	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.643	344.33	-5.209	6.46	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.802	343.35	-0.689	6.98	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.817	342.72	-3.826	6.91	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.806	344.33	-1.732	6.96	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.811	342.86	-2.642	6.94	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
CO <i>s-cis</i>	$\sigma$	0.943	1645.91	3.373	2.60	11	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub>
	$\sigma^+$	0.817	1646.15	2.231	2.66	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.713	1645.03	3.795	2.74	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.835	1647.39	3.941	2.70	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.827	1645.24	2.953	2.78	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.834	1647.42	3.385	2.71	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
CO <i>s-trans</i>	$\sigma$	0.730	1597.31	18.851	22.22	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.534	1598.24	15.971	21.09	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.830	1582.03	19.583	48.80	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.813	1597.71	-11.706	23.15	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.858	1579.19	51.448	18.75	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.811	1597.81	-9.011	23.20	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
CH <sub>ip</sub>	$\sigma$	0.862	1133.00	-36.031	16.97	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.871	1131.28	-30.670	15.24	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.712	1133.72	-17.739	27.39	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.859	1115.39	-49.652	17.50	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.806	1129.04	-4.875	21.77	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.806	1113.33	-48.880	16.27	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
CH <sub>op</sub>	$\sigma$	0.728	853.10	11.872	15.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.835	853.59	10.894	14.76	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.833	846.80	21.904	14.86	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.801	855.06	0.0411	15.77	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.838	845.68	22.704	14.52	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.803	855.57	1.761	15.76	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
CH=CH <sub>op</sub>	$\sigma$	0.704	1058.00	2.455	18.96	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.725	1085.56	-1.098	18.97	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.822	1051.76	17.608	18.50	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.816	1061.95	11.700	18.73	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.810	1056.66	5.681	18.92	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.817	1061.68	11.492	18.67	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
C=C <sub>op</sub>	$\sigma$	0.711	547.22	-6.381	21.77	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.613	572.98	1.301	21.40	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.816	567.69	14.501	21.12	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.940	565.49	-32.750	19.61	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.821	566.49	16.711	20.93	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.836	565.66	-26.400	19.99	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>

r = Correlation co-efficient;  $\rho$  = Slope; I = Intercept; s = Standard deviation; n = Number of substituents.

**Table 4. NMR spectral data of substituted styryl 2-pyrrolyl ketones.**

Entry	X	<sup>1</sup> H NMR δ(ppm)			<sup>13</sup> C NMR δ(ppm)			
		H <sub>α</sub> (d, 1H)	H <sub>β</sub> (d, 1H)	Substt.	CO	C <sub>α</sub>	C <sub>β</sub>	Substt.
1	H	7.10	7.84	---	178.93	122.04	142.25	---
2	2-Cl	7.16	7.69	---	177.98	126.42	140.42	---
3	3-Cl	7.11	7.74	---	177.42	125.81	140.83	---
4	4-Cl	7.09	7.76	---	178.31	126.92	141.24	---
5	3-F	7.19	7.83	---	179.48	126.35	141.31	---
6	4-F	7.29	7.85	---	178.65	125.17	141.01	---
7	2-OCH <sub>3</sub>	7.25	7.79		178.82	121.45	141.72	
8	3-OCH <sub>3</sub>	7.27	7.82		178.86	120.97	142.22	
9	4-OCH <sub>3</sub>	7.27	7.83		179.08	119.71	142.08	
10	4-CH <sub>3</sub>	7.31	7.80		178.99	125.04	142.35	
11	3-NO <sub>2</sub>	7.44	7.84	---	177.84	122.26	139.26	---
12	4-NO <sub>2</sub>	7.38	7.79	---	177.82	122.38	140.24	---

**Table 5. Results of statistical analysis of <sup>1</sup>H NMR of δH<sub>α</sub>, δH<sub>β</sub> (ppm), <sup>13</sup>C NMR of δC<sub>α</sub>, δC<sub>β</sub> and δCO (ppm) of substituted styryl 2-pyrrolyl ketones with Hammett σ, σ<sup>+</sup>, σ<sub>I</sub>, σ<sub>R</sub> constants and F and R parameters.**

Functionality	Const.	r	I	ρ	s	n	Correlated derivatives
δH <sub>α</sub> (ppm)	σ	0.728	7.221	0.008	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sup>+</sup>	0.716	7.231	0.033	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>I</sub>	0.827	7.184	0.133	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>R</sub>	0.825	7.264	0.111	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.831	7.183	0.132	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.816	7.251	0.165	0.11	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
δH <sub>β</sub> (ppm)	σ	0.821	7.800	-0.015	0.05	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sup>+</sup>	0.814	7.801	-0.021	0.04	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>I</sub>	0.814	7.809	-0.030	0.04	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>R</sub>	0.706	7.919	-0.011	0.05	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.845	7.791	-0.051	0.05	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.818	7.781	-0.034	0.04	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
δCO(ppm)	σ	0.963	178.69	-1.090	0.51	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sup>+</sup>	0.593	178.62	-0.777	0.53	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>I</sub>	0.753	179.06	-1.451	0.55	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>R</sub>	0.751	178.18	-1.423	0.54	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.823	178.76	-0.616	0.63	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.862	178.11	-1.390	0.51	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
δC <sub>α</sub> (ppm)	σ	0.836	123.44	1.624	2.50	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sup>+</sup>	0.727	123.51	1.402	2.51	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>I</sub>	0.826	122.61	2.981	2.51	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>R</sub>	0.854	123.70	-0.051	2.61	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.829	122.52	2.817	2.49	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.729	123.82	0.392	2.60	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
δC <sub>β</sub> (ppm)	σ	0.981	141.52	-2.105	0.59	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sup>+</sup>	0.906	141.43	-1.535	0.72	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>I</sub>	0.985	142.58	-3.561	0.51	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	σ <sub>R</sub>	0.741	140.81	-1.815	0.87	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.992	142.17	-1.270	0.75	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.832	144.18	-2.170	0.81	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>

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

**Table 6. The Reduction potential(v) and currents (i) of C=C and CO of substituted styryl 2-pyrrolyl ketones**

Entry	X	C=C(v)	C=C(i)	CO(v)	CO(i)
1	H	0.72	0.101	-0.65	-8.17
2	2-Cl	-0.241	1.382	-1.028	-6.85
3	3-Cl	0.74	3.178	-0.404	1.533
4	4-Cl	-0.26	1.321	-0.905	-2.455
5	3-F	-0.041	0.024	-0.397	1.381
6	4-F	0.643	0.026	-0.796	-8.083
7	2-OCH <sub>3</sub>	0.596	-0.04	0.861	6.891
8	3-OCH <sub>3</sub>	-0.167	-7.324	-0.508	-3.448
9	4-OCH <sub>3</sub>	0.805	0.363	0.029	-1.256
10	4-CH <sub>3</sub>	0.722	-2.413	-8.09	4.232
11	3-NO <sub>2</sub>	0.496	1.961	0.653	-7.913
12	4-NO <sub>2</sub>	0.57	1.954	-0.296	-3.455

**Table 7. Results of statistical analysis of reduction potential(v), current(i) of C=C and CO of substituted styryl 2-pyrrolyl ketones with Hammett substituent constants  $\sigma$ ,  $\sigma^+$ ,  $\sigma_I$ ,  $\sigma_R$  and F and R parameters**

Function	Constants	r	$\rho$	I	s	n	Correlated Derivatives
C=C (v)	$\sigma$	0.815	-0.185	3.634	0.43	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.837	-0.287	0.324	0.44	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.812	-0.283	0.442	0.47	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.807	0.102	0.357	0.47	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.823	-0.365	0.458	0.46	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.808	-0.095	0.311	0.47	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
C=C(i)	$\sigma$	0.941	4.111	0.114	0.28	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.928	1.149	0.761	0.31	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.906	9.219	2.724	2.54	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_R$	0.826	-2.897	0.167	3.14	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.902	0.371	0.794	3.24	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.909	2.978	1.547	2.97	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
C=O(v)	$\sigma$	0.831	1.716	-1.163	2.12	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.827	1.026	-0.876	2.13	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.811	1.666	-1.541	2.20	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.850	0.413	-1.061	2.22	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.816	0.974	-0.641	2.18	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
C=O(i)	$\sigma$	0.840	-5.208	-2.031	4.45	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma^+$	0.820	-2.224	-2.861	4.87	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	$\sigma_I$	0.811	-0.317	-2.671	5.07	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 2-NO <sub>2</sub> , 3-NO <sub>2</sub>
	$\sigma_R$	0.800	0.590	-2.751	5.07	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	F	0.828	4.714	-4.321	4.56	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>
	R	0.937	-4.330	-4.001	4.73	12	H, 2-Cl, 3-Cl, 4-Cl, 3-F, 4-F, 2-OCH <sub>3</sub> , 3-OCH <sub>3</sub> , 4-OCH <sub>3</sub> , 4-CH <sub>3</sub> , 3-NO <sub>2</sub> , 4-NO <sub>2</sub>

r=Correlation coefficient;  $\rho$ = Slope; I=Intercept; s= Standard deviation; n= Number of substituents.**Table 8. Antibacterial activity of substituted styryl 2-pyrrolyl ketones**

S.NO.	X	Zone of Inhibition (mm)				
		Gram positive Bacteria			Gram negative Bacteria	
		<i>K.pneumoniae</i>	<i>S.aureus</i>	<i>E.coli</i>	<i>B.subtilis</i>	<i>Micrococcus</i>
1	H	7	7	7	8	7
2	2-Cl	6	-	6	6	-
3	3-Cl	8	-	-	6	6
4	4-Cl	8	6	7	7	7
5	3-F	6	7	7	8	8
6	4-F	7	-	12	7	6
7	2-OMe	7	8	8	9	10
8	3-OMe	8	6	6	7	8
9	4-OMe	6	7	-	6	6
10	4-Me	7	7	-	8	7
11	3-NO <sub>2</sub>	6	6	7	10	8
12	4-NO <sub>2</sub>	8	7	6	12	6
Standard	Ampicillin	12	12	14	16	16
Control	DMSO					

Table 9. Antifungal activities of substituted styryl 2-pyrrolyl ketones

S.NO.	X	Zone of Inhibition (mm)		
		<i>A.niger</i>	<i>M.spp</i>	<i>T.viride</i>
1	H	7	10	9
2	2-Cl	6	6	6
3	3-Cl	-	6	-
4	4-Cl	6	12	9
5	3-F	6	8	8
6	4-F	7	-	-
7	2-OMe	-	-	-
8	3-OMe	6	7	6
9	4-OMe	7	8	6
10	4-Me	6	10	9
11	3-NO <sub>2</sub>	6	-	-
12	4-NO <sub>2</sub>	-	6	7
Standard	Miconazole	9	13	14
Control	DMSO			