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Solvent Free Synthesis, UV, IR spectral studies and Antimicrobial activities of some 2-[(*E*)-3-Substituted Phenylacryloyl] Cyclopentanones

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ABSTRACT

A series containing ten2-((*E*)-3-substituted phenylacryloyl) cyclopentanones have been synthesized bygreenaldol condensation. The absorption maxima (nm) λ_{max} and infrared stretches v(cm⁻¹) of CO_(s-cb) CO_(s-trans), deformations modes of CH_{ip}, _{op}, CH=CH_{op} and C=C_{op} were measured from their spectra. These frequencies were correlated with Hammett substituent constants and F and R parameters. From the results of statistical analyses the effects of substituents on the group frequencies can be explained. The antimicrobial activities of these synthesized chalcones have been studied using standard Bauer-Kirby method.

Keywords: 2-((*E*)-3-substituted phenylacryloyl) cyclopentanones, UVspectra, IR spectra, Hammett substituent constants, Regression analysis, Antimicrobial activities.



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INTRODUCTION

Spectral data of organic compounds are useful for prediction of structure, stereo chemical and physicochemical properties. There is considerable information avail in literature concerning the transmission of electronic effects in molecule undergoing isomer equilibration in ground state. For example enol and enones, α , β -unsaturated ketones[1] exist as s-cis and strans isomers which are confirmed by IR spectral data of equilibration in ground state. For example enol and enones, α , β -unsaturated ketones [1] exist as *s*-*cis* and *s*-*trans* isomers which are confirmed by IR spectroscopy. Mulliken [2] investigated the physicochemical properties of above system including those of polyenes and he absorbed equilibrium mixture of almost planar conformers. Several investigations have been shown that infrared wave number shift of mass intensities, stretches can be correlated with inductive and mesomeric effects [3] and other important physical properties [4] including empirical correlation [5]. The α , β unsaturated ketones possess multi-prolonged biological activities due to they possess methylene structural moieties[6]. The bio-activity data of such compounds were correlated for studying the quantitative structure activity and quantitative structure property relationships. Scientists and chemists were studied the effects of substituent by correlated the group frequencies of various ketones, epoxides with Hammett constants and F and R parameters using single and multi-regression analysis. There is no report on the study of effects of substituent on 2-((E)-3-substituted phenylacryloyl) cyclopentanones from literature. Hence the authors have taken efforts to synthesis cyclopentanonechalcones using greener catalyst and studied the effects of substituents on ultraviolet absorption and infrared group frequencies. The antimicrobial activities of all synthesized chalcones have been studied using Bauer-Kirby[7] method.

MATERIALS AND METHODS

General

Fly ash was collected from Thermal Power Plant–II, Neyveli Lignite Corporation (NLC), Neyveli, Tamilnadu, India. All chemicals used were purchased from Sigma-Aldrich and E-Merck chemical company. Melting points of all ω -bromo ketones were determined in open glass capillaries on Mettler FP51 melting point apparatus and are uncorrected. Further the purities of these ketones were checked by their spectral data published earlier in literature. Electron impact (EI) (70 eV) and chemical ionization mode FAB⁺ mass spectra were recorded with a VARIAN 500 spectrometer.

Experimental

General procedure for synthesis substituted styryl 2-pyrrolyl ketones[8]

In a 100ml flask, 2-acetyl pyrrole (4.16mmol) in aqueous ethanol (20ml), 1.5 g of fly-ash and 10 mL of water were taken. This flask was refluxed for 6 h (Scheme 1). The completion of reaction was monitored by TLC. After completion of the reaction the 2-pyrroylyl

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chalconeswere separated by column chromatogram using ethyl acetate-dichloromethane (6:4) gave the pale yellow products of 2-pyrroylyl chalcones , more than 70% yield. The analytical and spectral data of all synthesized 2-pyrroylyl chalcones are presented in Table 1.



Х	H 3-Br	2-Cl	3-Cl	3-F	4-F	3-OH	4-0CH ₃	4-CH ₃	3-NO ₂
					Scheme	1			

Table 1. Analytical, UV λ max(nm) and MS spectral data of 2-((*E*)-3-substituted phenylacryloyl) cyclopentanones

Entry	Х	M. F.	M.W	m.p.(°C)	λmax	MS(m/z)
1	Н	$C_{14}H_{12}O$	196	131	232	196[M ⁺], 119, 106, 93, 90, 77, 65, 27, 26
2	3-Br	$C_{14}H_{11}BrO$	275	156-157	235	275[M ⁺], 277[M ²⁺], 208, 195, 180, 168, 155,
						119, 106, 93, 78,77, 65
3	2-Cl	C ₁₄ H ₁₁ ClO	230	137-138	237	230[M ⁺], 232[M ²⁺], 195, 165, 155, 119, 111,
						106, 93, 77, 65
4	3-Cl	C ₁₄ H ₁₁ ClO	230	162-163	233	230[M ⁺], 232[M ²⁺], 195, 165, 155, 134, 124,
						119, 111, 106, 93, 77, 65, 34,
5	3-F	$C_{14}H_{11}FO$	214	141-142	222	214[M ⁺], 216[M ²⁺], 195, 165, 155, 149, 134,
						121, 119, 111, 108, 106, 95, 93, 77, 65, 54,
						34, 27, 19
6	4-F	$C_{14}H_{11}FO$	214	110-111	231	214[M ⁺], 216[M ²⁺], 195, 165, 155, 149, 134,
						121, 119,108, 93, 77, 65, 34,19
7	3-OH	$C_{14}H_{12}O_2$	212	171-172	224	212[M ⁺], 195, 147, 119, 93, 77, 65, 17
8	2-0CH ₃	$C_{15}H_{14}O_2$	226	121-122	241	226[M ⁺], 195, 161, 133, 119,120, 107, 106, 93,
						91, 77, 65, 31
9	4-CH ₃	$C_{15}H_{14}O_2$	210	121-122	235	210[M ⁺], 195, 145, 133, 119,117, 107, 106, 93,
						91, 77, 65, 15
10	3-NO ₂	$C_{14}H_{11}NO_3$	241	112-113	223	241[M ⁺], 195, 176, 148, 135, 122, 119, 106,
						93, 77, 65, 46

RESULTS AND DISCUSSION

There are number of solvent assisted C-C bond formatiom reactions available in literature for aldolcondensation. In the present work the authors have try to synthesised 2-pyrrolyl chalcones using crossed-aldol reaction between 2-acetyl pyrrole, substituted benzaldehydes and aqueous phase catalyst Fly-ash which are harmless to environment. Different 2-pyrrole ketones containing electron withdrawing groups and electron donation groups in sixth position are subjected to condensation on methyl groups within the presence of Fly-ash: water catalyst under solvent free conditions **(Scheme 1).** The yield and analytical data are presented in Table 1. The reaction was completed within 1h and good yields of 2-pyrrolyl



chalconesare obtained. Under these conditions it was observed that there is no dimerization occurring.

A waste air-pollutant Fly ash has many chemical species[9] SiO_2 , Fe_2O_3 , Al_2O_3 , CaO, MgO and insoluble residues. During the course of the reactions these species involve the promoting effects of condensation of methyl group with aldehydic groups. In these experiments the products were isolated and the catalyst was disposed by filtering. Further usage as catalyst is found to be ineffective. In this protocol the reaction gave good yields of the products, during condensation without any environmental discharge.

UV Spectral study

The UV spectra of all synthesisedchalcones were recorded in SHIMADZU-1650 SPECTROMETER (λ_{max} nm) in spectral grade methanol. The measure absorption maxima (λ_{max} nm) of these chalcones are presented in Table 1. 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

 $\lambda = \rho \sigma + \lambda_0$

...(1)

where λ_0 is the frequency for the parent member of the series.



Figure 1. The s-cis and s-trans conformers of substitutedstyryl 2-cyclopentanoketones

The results of statistical analysis of these values with Hammett substituent constants are presented in Table 3. From Table 3, Hammett substituent constants σ , σ^+ , σ_R and F values gave satisfactory correlations excluding 2-Cl, 3-Cl, 3-F, 3-OH and 4-CH₃ substituents. If they are included in the regression they reduce the correlation considerably. All constants gave positive ρ values however they produce satisfactory correlation. The σ_1 constant fails in correlation. This is due to the inductive effects of the substituents were weak for predicting the reactivity on the absorption. This evident with resonance conjugative structure shown in Figure 1. The multi regression analysis of these frequencies of all ketones with inductive, resonance and Swain – Lupton's[11] constants produce satisfactory correlations as evident in equations 2 and 3.



$$\lambda_{max}$$
 (nm) = -12.816(±0.671) σ_1 + 15.366(±2.084) σ_R + 235.49(±9.354) --- (2)
($R = 0.935$, P>90%, n=10)

$$\lambda_{max}$$
 (nm) = -14.937(±1.575)F +18.040 (±0.010)R+ 239.98(±7.697) --- (13)
(R = 0.963, P>95%, n=10)

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. 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[11]by single and multi linear regression analysis[8,12, 13]. While seeking Hammett correlation involving group frequencies, the form of the Hammett equation employed is

$$v = \rho \sigma + v_o \tag{4}$$

where v_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-3. From Table 3, the s-*cis* and s-*trans* conformers the correlation of $v_{C=0}$ with Hammett σ^+ values seem to be better. The s-*cis* carbonyl stretches (cm⁻¹) with R values give satisfactory correlation excluding 3-Br, 4-Me and 3-NO₂substituents in styryl moiety. The correlations with other sigma constants and F parameters give poor correlation co-efficient. This is due the conjugation between the substituent and the carbonyl group in chalcones as shown in Figure 2.



In view of the inability of some of the σ constants to produce individually satisfactory correlations, it was thought that worthwhile to seek multiple correlations involving either σ_{I} and σ_{R} constants or Swain-Lupton's[11], F and R parameters. The correlation equations for s-*cis* and s-*trans* are given equations 5-8.

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$$vCO_{s-cis}(cm^{-1}) = 14.529(\pm 2.895)\sigma_1 + 14.320(\pm 3.210)\sigma_R + 1638.94(\pm 13.408)--- (5)$$

(R = 0.922, P>90%, n=10)

$$vCO_{s-cis}(cm^{-1}) = 5.138(\pm 2.983))F+ 19.391 (\pm 1.562)R+ 1645.88(\pm 72.071) --- (6) (R = 0.941, P>90\%, n=10)$$

$$vCO_{s-trans}(cm^{-1}) = -2.122(\pm 2.801)\sigma_1 - 3.086 (\pm 3.120)\sigma_R + 1608.48(\pm 13.107) --- (7)$$

(R = 0.904, P>90%, n=10)

 $vCO_{s-trans}(cm^{-1}) = 2.272 (\pm 2.381) F + 12.091 (\pm 1.562) R+ 1611.82 (\pm 12.071) --- (8) (R = 0.927, P>90\%, n=10)$

The infrared spectra recorded in the present investigation for study the substituent effects on the deformation modes of C-H, CH=CH *out of plane, in-plane* and >C = C< *out of plane* vinyl parts of the chalcones. 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. The observed -CH = CH- and the CH frequencies in the present study are given in Table 2.

All the deformation modes of 2-((E)-3-substituted phenylacryloyl) cyclopentanones are correlated with different substituent constants according to Thirunarayanan and Jaishankar[14]. The results of statistical analysis are shown in Table 3.

The correlation of –CH *ip* deformation stretches with σ , σ^+ , σ_1 and F and R parametrs seems to be good excluding 3-OH, 2-OMe and 3-NO₂ substituents. The correlation of σ_R constant is quite bad. This is due to the fact that these values are not capable of predicting the substituent effects on CH *ip* vibrations.

Entry	Х	CO _(s-cis)	CO _(s-trans)	CH _{ip}	CH _{op}	CH=CH _{op}	C=C _{op}	Substituent styryl
				-				part
1	Н	1656.7	1625.9	1176.5	761.8	1070.4	516.9	
2	3-Br	1626.3	1598.4	1178.4	767.6	1029.9	594.0	
3	2-Cl	1664.5	1616.2	1180.4	754.1	1041.5	540.0	
4	3-Cl	1656.7	1604.7	1182.3	781.1	1093.6	563.2	
5	3-F	1647.1	1635.3	1182.3	781.1	1064.6	597.9	
6	4-F	1625.9	1589.2	1180.4	781.1	1012.6	518.8	
7	3-OH	1618.2	1585.4	1167.3	789.4	1025.7	525.4	3465.3(OH)
8	2-0CH ₃	1647.1	1627.8	1172.6	763.2	1029.9	530.4	1248.2(C-O-C)
9	4-CH ₃	1618.2	1595.0	1172.6	765.7	1016.4	522.7	
10	3-NO ₂	1638.3	1606.6	1184.2	736.8	1099.3	534.2	-

Table 2.Infrared spectral data v(cm⁻¹) of 2-((E)-3-substituted phenylacryloyl) cyclopentanones.

All correlations produce positive ρ values. This shows that normal substituent operates reversed in all systems, excluding F values. The failure correlations due to complete dies off resonance effect of substituent. Some of the single parameter correlations were not



worthwhile, while it will seek worthful in multi regression analysis [15] with F and R parameters and they produce the equations 9 and 10.

vCHip(cm⁻¹) = 17.695(±5.321)
$$\sigma_1$$
+9.211 (±5.912) σ_R + 1173.56 (±22.493) --- (9)
(R = 0.979, P>95%, n=10)
vCHip(cm⁻¹) = 15.231 (±2.284)F +9.605 (±1.526) R+ 1175.131(±11.524) --- (10)
(R = 0.995, P>99%, n=10)

The observed CHop frequencies in the present study are given in Table 2. All the deformation CHop modes of stretching frequencies of 2-((E)-3-substituted phenylacryloyl) cyclopentanones are correlated with different substituent constants. The results of statistical analysis are shown in Table 3.

From the table 3, correlation of CH*op* modes with Hammett σ^+ and R parameters seems satisfactory excluding 4-F substituent. All other singles correlations fail in this mode of frequencies with inductive, F and R parameters using single regression analysis. This is due to the reasons stated earlier in carbonyl frequencies along with conjugative structure shown in Figure 2. Some of the single correlations fail and hence it is thought worthwhile while seeking multi-regression analysis and the correlation equations are 11 and 12.

vCHop(cm⁻¹) = -13.214(±16.946) σ_1 - 56.065(±18.065) σ_R + 759.724(±7.850) --- (11) (R = 0.974, P>95%, n=10)

vCHop(cm⁻¹) = $-1.684(\pm 14.890)$ F $-29.809(\pm 9.809)$ R+ 757.838(± 7.552) --- (12) (R = 0.975, P>95%, n=10)

The observed -CH = CH- *op* frequencies in the present study are given in Table 2. All the frequencies of deformation modes of 2-((E)-3-substituted phenylacryloyl) cyclopentanones are correlated with different substituent constants. The results of statistical analysis are shown in Table 3.

The correlation of -CH = CH- *out of plane* deformation modes with σ_1 parameter seems to be satisfactory excluding H and 4-F substituents. The correlation with other σ constants and F and R values is quite bad. This is due to the fact that these values are not capable of predicting the substituent effects on -CH = CH- *out of plane* vibrations and the resonance effect of substituents completely dies off. This is shown in the conjugative structure Figure 2in which the π -bond character is converted into sigma character.

Some of the single parameter correlations were not worthwhile, while it will seek worthful in multi regression analysis with F and R parameters and they produce the equations 13 and 14.

vCH=CHop(cm⁻¹) = 59.552(\pm 35.741) σ_1 +95.795 (\pm 39.681) σ_R +1049.69 (\pm 16.556) ---(13)

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vCH=CHop(cm⁻¹) = 31.377(±36.538)F+45.271 (±24.413)R+ 1052.52 (±18.520) --- (14) (R = 0.902, P>90%, n=11)

The observed >C = C < op frequencies in the present study are given in Table 2. All the frequencies of deformation modes of substituted styryl 2-cyclopentano ketones are correlated with different substituent constants. The results of statistical analysis are shown in Table 3.

The correlation of >C = C< out of plane deformation modes with σ parameter seems to be satisfactory excluding 3-F and 3-NO₂ substituents. If they are included in the regression, they reduce the correlation considerably. The correlation with σ_{I} , σ_{R} , F 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 dies off. More over the polar effect of the substituents are also fails for prediction of the relativities on the π -bonds in theses chalcones. This is shown in the conjugative structure in Figure 2. in which the pi-bond character is converted into sigma character. Some of the single parameter correlations were not worthwhile, while it will seek worthful in multi regressionanalysis with F and R parameters and they produce the equations 15 and 16.

v>C = C< op (cm⁻¹) = 50.360(±43.320)
$$\sigma_1$$
-19.667(±48.110) σ_R +519.309 (±20.076)--- (15) (R = 0.948, P>90%, n=10)

$$v>C = C < op (cm^{-1}) = 53.234(\pm 38.651)F + 7.549(\pm 25.825)R + 525.757 (\pm 19.599) --- (16) (R = 0.946, P>90%, n=10)$$

Microbial activities

Chalconespossessa wide range of biological activities. These multipronged activities associated with different keto epoxides are intended to examine their above activities against respective microbes, fungi strains.

Antibacterial activity

The antibacterial activities of all the prepared chalcones have been evaluated against two gram positive pathogenic strains *Staphylococcus aureus*, *Enterococcus faecalis* while *Escherichia coli*, *Klebsiella*species, *Psuedomonas* and *Proteus vulgaris* were the gram negative strains. The disc diffusion technique was followed using the Kirby-Bauer[7]method, at a concentration of 250µg/mL with Ampicillin and Streptomycin used as the standard drugs. The measured antibacterial activities of all ketones are presented in Table 5. Against *Escherichia coli*, two compounds **2,3** and **7** showed maximum zone of inhibition with greater than 20 mm. The epoxides2, **3** and **7** were active against *Staphylococcus*, showing maximum inhibition. The other ketones showed less effective against *S. aureus*. The oxirane derivative **7** is more active against *Pseudomonas* at greater than 20mm zone of inhibition and the other derivatives inhibit

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the growth of bacterial between 12-19 mm zone of inhibitions. The epoxides **2** and **3** are effective against *Klebsiella* in 20-24 mm zone of inhibition while the other chalcones showed a moderate activity. The ketones **2-9** are active when they were screened against *P. vulgaris* and the other compounds are less effective. The ketones **2,3** and **9** showed moderate activities against *E.faecalis* when they were screened with 20-24 mm zone of inhibition.

Antifungal activity

Measurement of antifungal activities of all chalconeshave been done using *Candida albicans* as the fungal strain and the disc diffusion technique was followed for the antifungal activity while the two other strains *Penicillium* species and *Aspergillusniger*, the dilution method was adopted. The drugs dilution was 50µg/mL.*Griseofulvin*has been taken as the standard drug. The observed antifungal activities of all ketones are presented in Table 6.The study of antifungal activities of all ketones against*C. albicans*, showed that the two compounds 4 and 9 are effective at 20 mm as the zone of inhibition with 250µg/ disc while epoxides 7 and 8 are active at 13-19 mm zone of inhibition and the compounds 6 and7 are least active in 8-12 mm zone of inhibitions. Against *Penicillum* species, compound 4, 7 and 9 are visible while development of the fungal colony and 2-3 colonies are recorded for the compound 9. The inhibition of epoxides against *A.niger* was less in two compounds 4 and 7 being highly active followed by 8. Presence of a methoxy, methyl, and bromo substituents are responsible for antimicrobial activities of chalcones.

CONCLUSION

A series of ten substituted 2-*E*-(3-phenylacryloyl)cyclopentanones have been synthesised from greener method and they are characterized by their physical constants and UV-Vis and IR spectral data.From UV-Vis spectral data the maximum absorptions of all ketones were assigned and they are correlated with Hammett substituent constants and F and R parameter using single and multi-regression analysis. From the results of statistical analysis Hammett polar, Inductive and resonance and field effects were predicts their reactivity individually.

From IR spectra the carbonyl absorption of *s*-*cis* and *s*-*trans* conformers, deformation modes of vinyl part of the ketones such as CH*op/ip*, CH=CH*op*, and >C=C<*op* frequencies were assigned. They are correlated with various Hammett sigma constants and Swain-Lupton's parameters. The correlations of vCO*s*-*trans* conformers are less sensitive than *s*-*cis*. The correlations of CH*op/ip* deformation modes are satisfactory with Hammett σ , σ +, F and R parameters. A fair degree of correlation obtained from Hammett σ and σ_1 constants with CH=Ch*op*, >C=C<*op* deformation modes. All assigned group frequencies and deformation modes are responded with F and R and Swain-Lupton's constants using multi regression analysis.

From the antimicrobial study we found to be the compounds containing methoxy, methyl, and bromo substituent's are responsible for antimicrobial activities of chalcones.

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Table 3. The results of statistical analysis of absorption maxima (nm) and infrared group frequencies (v cm⁻¹) of substituted styryl 2-cyclopentanoketones with Hammett σ , σ^{\dagger} , $\sigma_{1,}\sigma_{R}$, F and R constants.

Frequency	Type of	r	ρ	I	S	n	Substituents in styryl part
Correlated	constants						
λmax(nm)	σ	0.901	5.967	226.26	1.43	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ^{+}	0.900	16.654	225.16	1.21	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and $3-NO_2$
	σ_1	0.800	-14.911	232.61	2.39	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_{R}	0.927	17.532	231.41	1.39	8	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.936	-18.674	234.80	1.34	8	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.801	19.424	234.48	4.76	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
CO _(s-cis)	σ	0.826	18.257	1637.64	18.18	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ^{+}	0.956	22.861	1637.80	4.88	8	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH,2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_1	0.819	12.595	1636.13	19.02	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH,2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_{R}	0.813	11.680	1643.54	19.10	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH $_3$, 4-CH $_3$, and 3-NO $_2$
	F	0.801	11.536	1640.34	19.27	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH $_3$, 4-CH $_3$, and 3-NO $_2$
	R	0.941	18.365	1647.77	7.17	8	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and $3-NO_2$
CO _(s-trans)	σ	0.805	1.039	1608.27	18.23	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and $3-NO_2$
	σ^{+}	0.938	1.485	1606.53	8.24	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and $3-NO_2$
	σ1	0.802	-1.703	1606.35	18.23	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_{R}	0.807	-2.698	1607.81	18.24	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.800	0.223	1608.36	17.63	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.827	11.839	1612.83	17.71	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
CH _{ip}	σ	0.962	13.452	1175.37	4.33	9	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ^{+}	0.961	8.188	1176.64	4.25	9	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_1	0.971	16.434	1171.84	4.00	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ_{R}	0.824	6.222	1179.16	5.52	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.965	13.242	1172.37	4.38	9	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.960	8.197	1180.73	4.55	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
CH _{op}	σ	0.855	-33.280	773.95	13.83	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ^{+}	0.965	-24.709	771.36	11.95	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ ₁	0.802	-5.541	770.16	16.54	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ _R	0.872	-53.850	756.54	11.58	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.780	4.488	766.38	16.55	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.970	-29.623	757.218	10.97	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
CH=CH _{op}	σ	0.864	78.135	1034.891	25.45	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂

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	σ^+	0.854	36.558	1043.69	28.74	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ1	0.934	46.443	1031.85	31.36	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ _R	0.857	85.740	1068.53	27.36	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.851	22.002	1039.54	32.84	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.853	42.371	1064.06	28.27	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
C=C _{op}	σ	0.931	36.391	538.04	30.46	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ^+	0.825	17.315	542.12	31.05	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ1	0.846	60.051	522.97	28.41	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	σ _R	0.820	-29.346	537.45	31.41	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	F	0.845	51.663	532.58	28.62	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂
	R	0.853	2.668	545.337	32.07	10	H, 3-Br, 2-Cl, 3-Cl, 3-F, 4-F, 3-OH, 2-OCH ₃ , 4-CH ₃ , and 3-NO ₂

Table 4. Antibacterial activity of of substituted styryl 2-cyclopentanoketones Entry

Entry	Х	E.coli	S.aures	Pseudomonas	Klebsiella	P.vulgaris	Enteroco ccus fae calis
1	Н	±	+	±	±	±	
2	3-Br	+	+	+	+	+	
3	2-Cl	+	+	+	+	+	
4	3-Cl	+	+	+	+	+	
5	3-F	++	++	++	+	+	
6	4-F	+	+	+	+	+	
7	3-OH	+	+	+	+	+	++
8	2-0CH ₃	+	+	+	+	+	++
9	4-CH ₃	±	+	±	±	±	
10	3-NO ₂	+	+	+	+	+	

Disc size: 6.35 mm; Duration: 24-45 h; Standard: Ampicillin (30-33 mm) and Streptomycin(20-25 mm); Control: Methanol; ---: No activities; ±: Active(8-12 mm); +: Moderately active(13-19 mm); ++: Active(20-24 mm).



Entry	Х	Disc diffusion technique(250µg/mL)	Drug dilution r	nethod (50µg/mL)
		Candida albicans	Penicillium	Aspergillusniger
1	Н	+		
2	3-Br	++	++	++
3	2-Cl		±	+
4	3-Cl	±		
5	3-F	±	++	++
6	4-F	+	+	+
7	3-OH	+	+	+
8	2-0CH ₃	++	++	+
9	4-CH ₃	+	+	
10	3-NO ₂	+	±	±

Table 5.Antifungal activity of of substituted styryl 2-cyclopentanoketones

Standard: Griseofulvinand Gentamycin; Duration : 72h; Control: Methanol; Medium: Potato dextrose agar; ++: No fungal colony; +: One fungal colony; ±: Two-three fungal colonies;---:Heavyfungalcolonies.

REFERENECES

- [1] Wang Y H, Zou J W, Zhang B, Lu Y X, Jin H X, Yu Q S. J MolStruct (Theochem) 2005; 755(1-2):31.
- [2] Mulliken R S. J ChemPhys 1939;7(2):121.
- [3] (a)Winecoff W F, Boykin D W Jr. J. Org. Chem.1973; 38(14):2544. (b) Paul WA S, Duyse A V. SpectrocimActa 1972; 28A(2):211.
- [4] DavisonW H T. J ChemSoc 1951; 2456. (b) Meda F. Spectrochim Acta1958; 13A(1-3):75.
- [5] Thirunarayanan G, Gopalakrishnan M, Vanangamudi G. SpectrochimActa 2007; 67(A):1106.
- [6] Thirunarayanan G. J Indian ChemSoc 2008; 85:447.
- [7] Bauer A W, Kirby W M M, Sherris J C, Truck M. Am J ClinPathol 1996; 45: 493.
- [8] Thirunarayanan G, Vanangamudi G, Sathiyendiran V. Ravi K.Indian J Chem 2011; 50(4):593.
- (a) Thirunarayanan G. Iup J Chem 2010; 3(4): 35. (b) Gopalakrishnan M, Sureshkumar P, Kanagarajan V, Thanusu J, Govindaraju R. Arkivoc 2006; 13: 130. (c) Gopalakrishnan M, Sureshkumar P, Kanagarajan V, Thanusu J. J Korean ChemSoc 2005; 51(6): 520.
- [10] Srinivasan S. 2002, Ph.D. Thesis. "Kinetics and Uv, IR and NMR spectral studies of some organic compounds".