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Synthesis and Hammett spectral QSAR analysis of some (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones

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ABSTRACT

About nine substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones have been synthesized by solvent-free method. These enones were analyzed by spectral techniques. The characteristic spectral frequencies were correlated through Hammett equation with Hammett substituent constants, F and R parameters using single and multi-regression analysis method. From the statistical analysis results, the quantitative structure activity relationships have been discussed by means of effects of substituents on the spectral frequencies.

Keywords: (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones, UV, IR, NMR spectra, QSAR study, regression analysis

1. INTRODUCTION

The basic structure of aryl α , β -unsaturated ketones includes two aromatic rings bound by an α , β -unsaturated carbonyl group, a unique template associated with very diverse application⁵.

Recently much attention has been paid on the synthesis of aryl α , β -unsaturated ketones mainly from acetophenones and various substituted aromatic aldehydes by Claisen-Schmidt condensation [1]. Aryl α , β -unsaturated ketones are products of condensation of simple or substituted aromatic aldehydes with simple or substituted acetophenones in the presence of alkali [2]. Compounds possessing such α , β -unsaturated carbonyl system have relatively low redox potentials and have a greater probability of undergoing electron transfer reactions [3]. By using different synthetic methods new derivatives of aryl α , β -unsaturated ketones were synthesized and characterized by physicochemical analysis in the recent past. Aryl α , β -unsaturated carbonyl system is an interesting nucleus for future developments in synthesizing effective compounds.

Microwave-assisted synthesis is an eco-friendly and efficient method of synthesis of organic compounds as compared to the conventional methods of synthesis [4-6]. The conventional methods require larger quantities of solvents and reagents and cause environmental pollution leading to the health hazards. Various methods available for synthesizing chalcones such as Aldol, Crossed-Aldol, Claisen-Schmidt, Knoevenagel, Greener methods-Grinding of reactants, solvent free and oxides of nanoparticles with microwave heating. Also microwave assisted solvent free Aldol and Crossed-Aldol condensation [7-9] were useful synthesis of carbonyl compounds. Microwave irradiation technique is a low cost and eco-friendly synthesis [10] giving high yields, in shorter reaction times. Recently, Christuraj *et.al.*, [11] synthesized the (*E*)-3-(5-bromothiophen-2-yl)-1-phenylprop-2-en-1-one compounds and explain the structure parameter study for (*E*)-3-(5-bromothiophen-2-yl)-1-phenylprop-2-en-1-one compounds.

Literature survey shows that there is no information available regarding the study of UV, IR and NMR spectral correlation of substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds. Hence the authors have taken efforts for the above spectral data of these (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds for studying the quantitative structure activity relationships through Hammett correlations.

2. EXPERIMENTAL

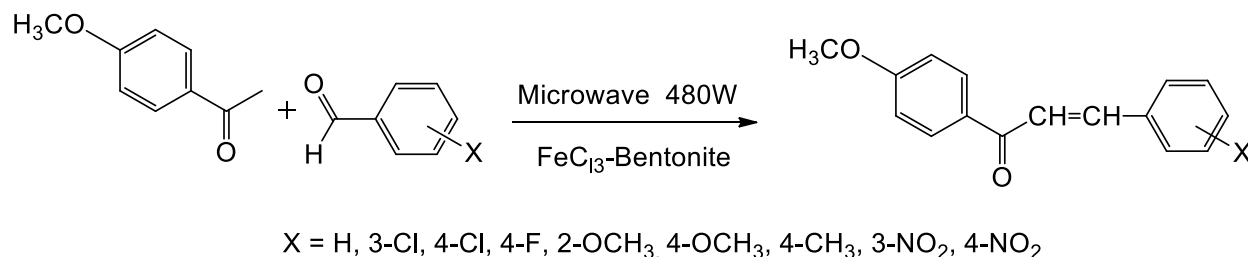
2. 1. Materials and Systematic methods

All chemicals purchased from Sigma-Aldrich chemical company Bangalore. All synthesized (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds melting points are observed from uncorrected Sutex melting point apparatus using open glass capillaries. The above chalcone compound analysed for Ultra violet spectra recorded using SHIMADZU-1650 SPECTROMETER. Infrared spectra (KBr, 4000-400 cm^{-1}) have been recorded on AVATAR-NICOLET 330 FT-IR spectrophotometer. BRUKER-400MHz NMR spectrometers has been operated for recording ^1H and ^{13}C spectra in CDCl_3 solvent using internal standard as TMS.

2. 2. General procedure for synthesis of (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones

Substituted styryl 4-methoxyphenyl ketones were synthesized by procedure reported in the literature [12]. An equal molar quantity of 4-methoxyacetophenone (0.01 mol) with substituted benzaldehydes (0.01 mol) and FeCl_3 -Bentonite [13] (0.4 g) catalyst were placed in a Borosil beaker and covered with watch glass. The reaction mixture has been irradiated to

microwave for 5–6 minutes (**Scheme 1**) (IFB Microwave Oven, 480 W) and then wait for this mixture attain to room temperature (30 °C). The extraction of organic layer with dichloromethane and evaporation of solvent afforded the crude product. The insoluble catalyst was recycled by purified with ethyl ethanoate and heated in an hot air oven at 100 °C for 1 h. Recrystallization of crude product with benzene-hexane mixture to afforded pale yellow glittering solids. The synthesized (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones have been characterized by their physical constants, elemental analysis and spectral data. The characteristic spectroscopic data of all 4-methoxyphenyl chalcones were presented in Table 1.



Scheme 1. Synthesis of (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones

Table 1. The ultraviolet absorption maxima (λ_{max} , nm), infrared absorptions (ν , cm^{-1}) and NMR chemical shifts (δ , ppm) spectral data of substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones.

Entry	X	UV (nm) λ_{max}	IR (ν , cm^{-1})					
			CO <i>s-cis</i>	CO <i>s-trans</i>	CH _{ip}	CH _{op}	CH=CH _{op}	C=C _{op}
1	H	311.6	1653.59	1602.95	1183.46	762.05	1018.79	561.67
2	3-Cl	296.0	1664.44	1599.02	1168.57	777.69	1018.69	560.45
3	4-Cl	314.0	1652.00	1592.00	1184.65	820.00	1017.89	560.56
4	4-F	255.0	1654.78	1601.96	1185.28	821.89	1015.85	534.15
5	2-OCH ₃	343.0	1655.08	1595.18	1167.17	818.27	1016.27	528.19
6	4-OCH ₃	346.0	1653.91	1595.64	1168.67	818.98	1019.70	529.51
7	4-CH ₃	310.8	1648.48	1593.28	1170.20	812.82	1012.53	534.25
8	3-NO ₂	277.5	1663.82	1599.01	1170.96	868.75	1019.55	569.86
9	4-NO ₂	287.0	1668.28	1597.17	1175.59	832.75	1033.37	570.02

NMR chemical shifts (δ , ppm)								
Entry	X	H $_{\alpha}$	H $_{\beta}$	X	CO	C $_{\alpha}$	C $_{\beta}$	X
1	H	7.553	7.809	---	188.78	121.91	144.02	---
2	3-Cl	7.544	7.728	---	188.31	123.09	142.26	---
3	4-Cl	7.519	7.748	---	188.44	122.30	142.50	---
4	4-F	7.477	7.768	---	188.53	121.58	142.70	---
5	2-OCH $_3$	7.602	7.780	1.832	188.82	119.58	143.85	64.39
6	4-OCH $_3$	7.436	7.783	2.126	188.92	119.55	143.87	66.72
7	4-CH $_3$	7.513	7.790	3.014	188.89	120.86	144.12	26.91
8	3-NO $_2$	7.676	7.831	---	188.13	122.21	140.87	---
9	4-NO $_2$	7.238	7.772	---	195.12	123.81	146.54	---

3. RESULTS AND DISCUSSION

3. 1. Spectral linearity

In the current study the spectral linearity of synthesized (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones has been studied by evaluating the substituent effects. The observed spectral data for the (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones, UV λ_{\max} (nm), infrared CO *s-cis*, CO *s-trans*, CH $_{ip}$, CH $_{op}$, CH=CH $_{op}$, C=C $_{op}$, the proton chemical shifts δ (ppm) of H $_{\alpha}$, H $_{\beta}$ and carbon chemical shifts of C=O, C $_{\alpha}$, and C $_{\beta}$ are correlated with various substituent constants [13-17].

3. 1. 1. UV spectral study

The measured absorption maxima (λ_{\max} nm) values of the synthesized (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds have been recorded and presented in Table 1. These data are correlated with Hammett substituent constants and *F* and *R* parameters using single and multi-linear regression analysis [13-17]. Hammett equation employed for the correlation analysis, involving the absorption maxima is as shown below in equation (1).

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

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

The Hammett spectral correlation results of these data were presented in Table 2. From the Table 2, it is evident that the UV absorption maximum (λ_{\max} nm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds have shown satisfactory correlations with Hammett substituent constants σ ($r = 0.906$) and σ^+ ($r = 0.906$). However, the UV (λ_{\max} nm) values of (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have

shown poor correlation ($r < 0.900$) with remaining Hammett substituent constant σ_I , σ_R and F and R parameters. This is attributed to the weak inductive, field and resonance effects of substituents for predicting the reactivity on the UV absorption through resonance as per the conjugative structure as shown in Figure 1.

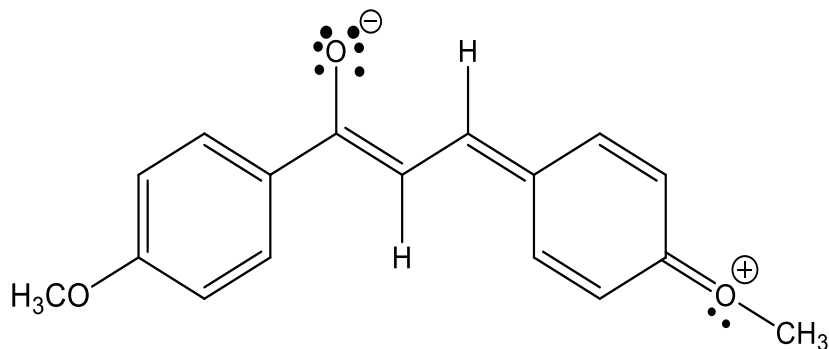


Figure 1. Resonance conjugative structure

Table 2. The results of statistical analysis of ultraviolet absorption maxima (λ_{max} , nm), infrared absorptions (ν , cm^{-1}) and NMR chemical shifts (δ , ppm) of substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones with Hammett σ , σ^+ , σ_I , σ_R and F and R parameters.

Freq.	Constt.	r	I	ρ	s	n	Correlated Derivatives
λ_{max}	σ	0.906	304.5	-98.550	95.34	8	H, 3-Cl, 4-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.906	290.9	-61.240	95.8	8	H, 3-Cl, 4-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_I	0.851	337.3	-123.818	96.42	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.831	279.05	-78.403	99.13	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	F	0.866	323.98	-74.271	99.2	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	R	0.735	285.84	-51.946	99.21	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
$\nu_{\text{CO}_{s-cis}}$ (cm^{-1})	σ	0.908	1655.23	12.967	4.12	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.900	1656.71	9.960	4.36	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_I	0.907	1650.06	19.390	4.78	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.848	1659.4	12.200	6.22	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂

	<i>F</i>	0.906	1651.07	15.760	5.51	7	H, 3-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>R</i>	0.905	1659.78	11.700	6.14	6	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂ , 4-NO ₂
$\nu_{\text{CO}_3\text{-trans}}$ (cm ⁻¹)	σ	0.784	1597.06	1.984	3.88	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.802	1597.27	1.980	3.82	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_{I}	0.801	1596.8	1.508	3.96	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_{R}	0.814	1597.22	1.978	3.94	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>F</i>	0.902	1596.25	2.845	3.89	7	H, 3-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>R</i>	0.801	1597.7	1.553	3.95	6	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂ , 4-NO ₂
$\nu_{\text{CH}_{\text{ip}}}$ (cm ⁻¹)	σ	0.900	1174.57	2.545	7.61	6	H, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ ,
	σ^+	0.900	1174.84	2.423	7.92	6	H, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃
	σ_{I}	0.707	1174.18	2.086	8.02	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_{R}	0.900	1175.49	2.964	7.99	6	3-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>F</i>	0.900	1173.11	4.751	7.92	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>R</i>	0.800	1175.43	2.178	8.01	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
$\nu_{\text{CH}_{\text{op}}}$ (cm ⁻¹)	σ	0.900	810.68	27.837	30.26	7	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.902	814.12	15.364	31.56	7	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_{I}	0.906	788.071	73.106	25.67	7	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_{R}	0.809	817.88	16.719	32.38	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>F</i>	0.900	787.49	70.817	25.67	6	4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	<i>R</i>	0.806	817.21	10.752	32.56	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂

$\nu_{\text{CH}=\text{CH}_{op}}$ (cm^{-1})	σ	0.966	1017.83	9.195	4.60	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ^+	0.905	1018.91	6.432	4.99	7	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ_I	0.900	1014.72	12.235	5.20	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ_R	0.905	1021.24	11.105	5.30	7	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂
	F	0.904	1015.51	9.531	5.54	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	R	0.905	1021.45	10.074	5.33	7	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂
$\nu_{\text{C}=\text{C}_{op}}$ (cm^{-1})	σ	0.908	544.32	37.388	9.09	7	3-Cl, 4-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.908	548.51	30.291	8.33	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_I	0.804	538.58	30.811	17.11	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.905	560.44	57.423	9.74	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂ , 4-NO ₂
	F	0.802	542.41	19.293	18.25	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	R	0.902	562.17	54.929	8.60	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 3-NO ₂ , 4-NO ₂
δH_{α} (ppm)	σ	0.902	7.516	-0.065	0.12	7	H, 3-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ^+	0.901	7.507	-0.027	0.12	7	H, 3-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ_I	0.801	7.539	-0.091	0.12	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.901	7.494	-0.065	0.12	7	H, 3-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	F	0.801	7.545	-0.100	0.12	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	R	0.907	7.499	-0.029	0.13	7	H, 3-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
δH_{β} (ppm)	σ	0.825	7.778	0.002	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.801	7.778	0.001	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_I	0.705	7.787	-0.024	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.706	7.786	0.040	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂

	<i>F</i>	0.705	7.786	-0.019	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>R</i>	0.706	7.786	0.033	0.03	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
δC_O (ppm)	σ	0.904	188.96	2.463	2.06	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ^+	0.904	143.30	-0.145	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ ,
	σ_I	0.901	143.53	-0.630	1.66	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ_R	0.806	143.36	0.354	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	<i>F</i>	0.801	143.55	-0.657	1.66	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	<i>R</i>	0.702	143.37	0.337	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
δC_α (ppm)	σ	0.981	121.20	3.059	0.72	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.961	121.54	2.506	0.62	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ_I	0.905	120.58	2.915	1.93	7	H, 3-Cl, 4-Cl, 4-F, 4-OCH ₃ , 3-NO ₂ , 4-NO ₂
	σ_R	0.907	122.38	3.965	1.06	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>F</i>	0.811	120.74	2.364	1.39	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	<i>R</i>	0.900	122.48	3.696	1.98	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
δC_β (ppm)	σ	0.903	143.32	-0.112	1.67	9	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ , 4-NO ₂
	σ^+	0.904	143.30	-0.145	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂ ,
	σ_I	0.901	143.53	-0.630	1.66	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	σ_R	0.806	143.36	0.354	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	<i>F</i>	0.801	143.55	-0.657	1.66	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
	<i>R</i>	0.702	143.37	0.337	1.67	8	H, 3-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 3-NO ₂
<p>r = Correlation co-efficient; ρ = slope; I = Intercept; s = Standard deviation; n = Number of substituents</p>							

All the correlations have shown negative ρ values. This indicates the reverse substituent effect with respect to UV absorption maximum (λ_{\max} nm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds. Some of the single parameter correlations failed for the UV absorption maximum (λ_{\max} nm) values with Hammett constants and *F* and *R* parameter, it is decided to go for multi regression analysis with Swain-Lupton's [18]. While pursuing the multi regression analysis there is satisfactory correlations are observed as shown in the following equations (2) and (3).

$$\lambda_{\max} (\text{nm}) = 317.32 (\pm 59.291) - 165.222 (\pm 130.806) \sigma_I - 80.574 (\pm 130.438) \sigma_R \quad \dots(2)$$

$$(R = 0.961, n = 9, P > 95\%)$$

$$\lambda_{\max} (\text{nm}) = 312.38 (\pm 55.783) - 83.453 (\pm 130.310) F - 58.398 (\pm 91.380) R \quad \dots(3)$$

$$(R = 0.973, n = 9, P > 95\%)$$

3. 1. 2. IR spectral study

The assigned infrared frequencies (cm^{-1}) of CO_{s-cis} , $\text{CO}_{s-trans}$, CH_{ip} , CH_{op} , $\text{CH}=\text{CH}_{op}$, and $\text{C}=\text{C}_{op}$ of substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ones are presented in **Table 1**. The measured infrared frequency values are correlated [14-17] with Hammett substituent constants and *F* and *R* parameters using single and multi-linear regression analysis. Hammett equation employed for the correlation analysis, involving the absorption maxima is as shown below in equation (4).

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

where ν_0 is the frequency for the parent member of the series.

3. 1. 2. 1. IR Spectral Correlation of νCO_{s-cis} (cm^{-1})

From the **Table 2**, it is evident that the IR frequency $\nu\text{C}=\text{O}$ (cm^{-1}) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds have shown satisfactory correlations with Hammett substituent constants σ ($r = 0.908$), σ^+ ($r = 0.900$), σ_I ($r = 0.907$). The IR $\nu\text{C}=\text{O}_{s-cis}$ (cm^{-1}) values for except those with 4-Cl and 4-F, have shown satisfactory correlation with *F* parameter ($r = 0.906$) only. The IR $\nu\text{C}=\text{O}_{s-cis}$ (cm^{-1}) values for except those with H (parent), 4-Cl and 4-F substituent have shown satisfactory correlation with *R* parameter ($r = 0.905$). The remaining Hammett substituent constant σ_R parameter has shown poor correlation ($r < 0.900$) with the σ_R . This is attributed to the weak resonance effect of substituents for predicting the reactivity on the IR frequency νCO_{s-cis} (cm^{-1}) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency νCO_{s-cis} (cm^{-1}) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 2. 2. IR Spectral Correlation of $\nu\text{CO}_{s-trans}$ (cm^{-1})

From the **Table 2**, it is evident that the IR frequency $\nu\text{CO}_{s-trans}$ (cm^{-1}) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 4-Cl and 4-F substituents have shown satisfactory correlation with *F* parameter ($r = 0.902$).

The remaining Hammett substituent constants σ , σ^+ , σ_I , σ_R and R parameter have shown poor correlation ($r < 0.900$). This is attributed to the weak polar, inductive and resonance effects of substituents for predicting the reactivity on the IR frequency $\nu\text{CO}_{s-trans}$ (cm^{-1}) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency $\text{CO}_{s-trans}$ (cm^{-1}) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 2. 3. IR Spectral Correlation of νCH_{ip} (cm^{-1})

From the **Table 3**, it is evident that the IR frequency νCH_{ip} (cm^{-1}) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 3-Cl, 3-NO₂ and 4-NO₂ substituents have shown satisfactory correlations with a few Hammett substituent constants namely σ ($r = 0.900$) and σ^+ ($r = 0.900$). The IR νCH_{ip} (cm^{-1}) values for except those with H (parent), 4-Cl and 4-F substituents have shown satisfactory correlation with the Hammett substituent constant σ_R ($r = 0.900$). The IR νCH_{ip} (cm^{-1}) values for satisfactory correlation with F parameter ($r = 0.900$).

The remaining Hammett substituent constant σ_I and R parameter have shown poor correlations ($r < 0.900$). This is attributed to the weak inductive and resonance effects of substituents for predicting the reactivity on the IR frequency νCH_{ip} (cm^{-1}) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency νCH_{ip} (cm^{-1}) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 2. 4. IR Spectral Correlation of νCH_{op} (cm^{-1})

From the **Table 3**, it is evident that the IR frequency νCH_{op} (cm^{-1}) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with H (parent) and 3-Cl, substituents have shown satisfactory correlations with Hammett substituent constants namely σ ($r = 0.900$), σ^+ ($r = 0.902$) and σ_I ($r = 0.906$). The IR νCH_{op} (cm^{-1}) values for except those with H (parent), 4-Cl, 4-F and 3-NO₂ substituents have shown satisfactory correlation with the F parameter ($r = 0.900$).

The remaining Hammett substituent constant σ_R and R parameter have shown poor correlations ($r < 0.900$). This is attributed to the weak resonance effects of substituents for predicting the reactivity on the IR frequency νCH_{op} (cm^{-1}) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency νCH_{op} (cm^{-1}) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 2. 5. IR Spectral Correlation of $\nu\text{CH}=\text{CH}_{op}$ (cm^{-1})

From the **Table 3**, it is evident that the IR frequency $\nu\text{CH}=\text{CH}_{op}$ (cm^{-1}) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except that with 4-NO₂ substituent have shown satisfactory correlations with Hammett substituent constants namely σ ($r = 0.966$), σ_I ($r = 0.900$) and F parameter ($r = 0.904$). The IR $\nu\text{CH}=\text{CH}_{op}$ (cm^{-1}) values

for except those with 4-CH₃ and 4-NO₂ substituents have shown satisfactory correlation with the Hammett substituent constant σ_R ($r = 0.905$) R parameter ($r = 0.905$).

The IR $\nu\text{CH}=\text{CH}_{op}$ (cm⁻¹) values for except those with 4-OCH₃ and 4-NO₂ substituents have shown satisfactory correlation with the Hammett substituent constant σ^+ ($r = 0.905$).

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency $\nu\text{CH}=\text{CH}_{op}$ (cm⁻¹) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 2. 6. IR Spectral Correlation of $\nu\text{C}=\text{C}_{op}$ (cm⁻¹)

From the **Table 3**, it is evident that the IR frequency $\nu\text{C}=\text{C}_{op}$ (cm⁻¹) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have shown satisfactory correlations with Hammett substituent constant σ^+ ($r = 0.908$). The IR $\nu\text{C}=\text{C}_{op}$ (cm⁻¹) values for except that with 4-CH₃ substituent have shown satisfactory correlations with Hammett substituent constants σ_R ($r = 0.905$) R parameter ($r = 0.902$). The IR $\nu\text{C}=\text{C}_{op}$ (cm⁻¹) values for except those with H (parent) and 4-F substituents have shown satisfactory correlations with Hammett substituent constant σ ($r = 0.908$).

The remaining Hammett substituent constant σ_I and F parameter have shown poor correlations ($r < 0.900$). This is attributed to the weak inductive and field effects of substituents for predicting the reactivity on the IR frequency $\nu\text{C}=\text{C}_{op}$ (cm⁻¹) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to IR frequency $\nu\text{C}=\text{C}_{op}$ (cm⁻¹) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

Some of the single parameter correlations analyses failed for the infrared frequencies (cm⁻¹) of CO_{*s-cis*}, CO_{*s-trans*}, CH_{*ip*}, CH_{*op*}, CH=CH_{*op*}, and C=C_{*op*} values of (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds with Hammett substituent constants and F and R parameter, it is decided to go for multi regression analysis with Swain-Lupton's [23] parameters. While seeking the multi regression analysis there is satisfactory correlations are observed as shown in the following equations (5) to (16).

$$\nu\text{CO}_{s-cis} (\text{cm}^{-1}) = 1652.39(\pm 2.980) + 17.7551(\pm 6.051)\sigma_I + 9.371(\pm 5.785)\sigma_R \quad \dots(5)$$

($R = 0.908$, $n = 9$, $P > 90\%$)

$$\nu\text{CO}_{s-cis} (\text{cm}^{-1}) = 1653.74(\pm 3.098) + 15.417(\pm 6.074)F + 11.303(\pm 5.621)R \quad \dots(6)$$

($R = 0.908$, $n = 9$, $P > 90\%$)

$$\nu\text{CO}_{s-trans} (\text{cm}^{-1}) = 1597.24(\pm 2.935) + 1.196(\pm 5.959)\sigma_I + 1.787(\pm 5.697)\sigma_R \quad \dots(7)$$

($R = 0.916$, $n = 9$, $P > 90\%$)

$$\nu\text{CO}_{s-trans} (\text{cm}^{-1}) = 1596.60(\pm 2.811) + 2.800(\pm 5.511)F + 1.480(\pm 5.101)R \quad \dots(8)$$

($R = 0.923$, $n = 9$, $P > 90\%$)

$$\nu\text{CH}_{ip} (\text{cm}^{-1}) = 1174.859(\pm 5.966) + 1.613(\pm 12.113)\sigma_I + 2.707(\pm 11.581)\sigma_R \quad \dots(9)$$

($R = 0.900$, $n = 9$, $P > 90\%$)

$$\nu_{\text{CH}_{ip}} (\text{cm}^{-1}) = 1173.603(\pm 5.739) + 4.688(\pm 11.250)F + 2.055(\pm 10.412)R \quad \dots(10)$$

(R = 0.900, n = 9, P > 90%)

$$\nu_{\text{CH}_{op}} (\text{cm}^{-1}) = 789.367(\pm 19.358) + 72.198(39.304)\sigma_I + 5.202(\pm 37.579)\sigma_R \quad \dots(11)$$

(R = 0.961, n = 9, P > 95%)

$$\nu_{\text{CH}_{op}} (\text{cm}^{-1}) = 789.599(\pm 18.546) + 70.544(\pm 36.353)F + 8.903(\pm 33.645)R \quad \dots(12)$$

(R = 0.962, n = 9, P > 95%)

$$\nu_{\text{CH}=\text{CH}_{op}} (\text{cm}^{-1}) = 1017.058(\pm 3.343) + 10.592(\pm 6.788)\sigma_I + 9.415(\pm 6.490)\sigma_R \quad \dots(13)$$

(R = 0.968, n = 9, P > 95%)

$$\nu_{\text{CH}=\text{CH}_{op}} (\text{cm}^{-1}) = 1017.841(\pm 3.365) + 9.230(\pm 6.597)F + 9.832(\pm 6.106)R \quad \dots(14)$$

(R = 0.966, n = 9, P > 95%)

$$\nu_{\text{C}=\text{C}_{op}} (\text{cm}^{-1}) = 551.995(\pm 5.876) + 21.386(\pm 11.931)\sigma_I + 54.012(\pm 11.407)\sigma_R \quad \dots(15)$$

(R = 0.991, n = 9, P > 95%)

$$\nu_{\text{C}=\text{C}_{op}} (\text{cm}^{-1}) = 555.280(\pm 5.060) + 17.626(\pm 9.920)F + 54.467(\pm 9.181)R \quad \dots(16)$$

(R = 0.993, n = 9, P > 95%)

3. 1. 3. NMR spectral study

In nuclear magnetic resonance spectra, the proton and the ¹³C chemical shifts (δ) depends on the electronic environment of the nuclei concerned. The assigned chemical shifts (ppm) have been correlated with reactivity parameters using Hammett equation [13-17] in the form of

$$\delta = \rho\sigma + \delta_o \quad \dots(17)$$

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

3. 1. 3. 1. ¹H NMR Spectral Correlation

3. 1. 3 .1. 1. ¹H NMR Spectral Correlations of δH_α (ppm)

From the **Table 2**, it is evident that the δH_α chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 2-OCH₃ and 4-NO₂, substituents have shown satisfactory correlations with Hammett substituent constants namely σ (r = 0.902), σ⁺ (r = 0.901), σ_R (r = 0.901) and R parameter (r = 0.907).

The remaining Hammett substituent constant σ_I and F parameter have shown poor correlations (r < 0.900). This is attributed to the weak inductive and field effects of substituents for predicting the reactivity on the δH_α chemical shift (ppm) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to δH_α chemical shift (ppm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 3. 1. 2. ^1H NMR Spectral Correlations of δH_β (ppm)

From the **Table 2**, it is evident that the δH_β chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have shown poor correlations ($r < 0.900$) with Hammett substituent constants and *F* and *R* parameters.

This is attributed to the weak polar, inductive, field and resonance effects of substituents for predicting the reactivity on the δH_β chemical shift (ppm) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values except σ_I and *F* parameter. This indicates the operation of normal substituent effect with respect to δH_β chemical shift (ppm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 3. 2. ^{13}C NMR Spectral Correlation

3. 1. 3. 2. 1. ^{13}C NMR Spectral Correlations of $\delta\text{C}=\text{O}$ (ppm)

From the **Table 2**, it is evident that the δCO chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have shown satisfactory correlations with Hammett substituent constants namely σ_R ($r = 0.904$), *F* ($r = 0.902$) and *R* ($r = 0.903$) parameters. The δCO chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except that with 4- NO_2 , substituent have shown satisfactory correlations with Hammett substituent constants namely σ ($r = 0.904$), σ^+ ($r = 0.904$), σ_I ($r = 0.903$).

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to δCO chemical shift (ppm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 3. 2. 2. ^{13}C NMR Spectral Correlations of δC_α (ppm)

From the **Table 2**, it is evident that the δC_α chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have shown satisfactory correlations with Hammett substituent constants namely, σ ($r = 0.981$), σ^+ ($r = 0.961$), σ_R ($r = 0.907$) and *R* ($r = 0.900$) parameter.

The δC_α chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 2- OCH_3 and 4- CH_3 , substituents have shown satisfactory correlations with Hammett substituent constants namely σ_I ($r = 0.905$).

The remaining *F* parameter has shown poor correlation ($r < 0.900$). This is attributed to the weak field effect of substituents for predicting the reactivity on the δC_α chemical shift (ppm) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to δC_α chemical shift (ppm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

3. 1. 3. 2. 3. ^{13}C NMR Spectral Correlations of δC_β (ppm)

From the **Table 2**, it is evident that the δC_β chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, have shown satisfactory correlations with Hammett substituent constant namely, σ ($r = 0.903$).

The δC_{β} chemical shift (ppm) values of all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds, except that with 4-NO₂, substituent have shown satisfactory correlations with Hammett substituent constants σ^+ ($r = 0.961$), σ_I ($r = 0.905$).

The remaining Hammett substituent constants σ_R , and *F* and *R* parameters have shown poor correlations ($r < 0.900$). This is attributed to the weak field and resonance effects of substituents for predicting the reactivity on the δC_{β} chemical shift (ppm) through resonance as per the conjugative structure as shown in **Figure 1**.

All the correlations have shown negative ρ values except σ_R , and *R* parameter. This indicates the operation of reverse substituent effect with respect to δC_{β} chemical shift (ppm) values in all substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds.

Some of the single parameter correlations analyses failed for the ¹H and ¹³C chemical shift (ppm) values of (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds with Hammett substituent constants and *F* and *R* parameter, it is decided to go for multi regression analysis with Swain-Lupton's [23] parameters. While seeking the multi regression analysis there is satisfactory correlations are observed as shown in the following equations (18) to (27).

$$\delta H_{\alpha} (\text{ppm}) = 7.526(\pm 0.095) - 0.082(\pm 0.193)\sigma_I - 0.052(\pm 0.184)\sigma_R \quad \dots(18)$$

(R = 0.924, n = 9, P > 90%)

$$\delta H_{\alpha} (\text{ppm}) = 7.538(\pm 0.092) - 0.099(\pm 0.181)F - 0.027(\pm 0.167)R \quad \dots(19)$$

(R = 0.922, n = 9, P > 90%)

$$\delta H_{\beta} (\text{ppm}) = 7.798(\pm 0.021) - 0.032(\pm 0.044)\sigma_I + 0.045(\pm 0.042)\sigma_R \quad \dots(20)$$

(R = 0.944, n = 9, P > 90%)

$$\delta H_{\beta} (\text{ppm}) = 7.794(\pm 0.022) - 0.020(\pm 0.043)F + 0.034(\pm 0.040)R \quad \dots(21)$$

(R = 0.933, n = 9, P > 90%)

$$\delta CO (\text{ppm}) = 189.07(\pm 1.528) + 2.227(\pm 3.103)\sigma_I + 3.030(\pm 2.967)\sigma_R \quad \dots(22)$$

(R = 0.948, n = 9, P > 90%)

$$\delta CO (\text{ppm}) = 189.13(\pm 1.489) + 2.218(\pm 2.919)F + 2.957(\pm 2.701)R \quad \dots(23)$$

(R = 0.948, n = 9, P > 90%)

$$\delta C_{\alpha} (\text{ppm}) = 121.48 (\pm 0.646) + 2.286(\pm 1.312)\sigma_I + 3.601(\pm 1.254)\sigma_R \quad \dots(24)$$

(R = 0.900, n = 9, P > 90%)

$$\delta C_{\alpha} (\text{ppm}) = 121.60 (\pm 0.599) + 2.252(\pm 1.174)F + 3.637(\pm 1.086) R \quad \dots(25)$$

(R = 0.984, n = 9, P > 95%)

$$\delta C_{\beta} (\text{ppm}) = 143.649 (\pm 1.241) - 0.711(\pm 2.520)\sigma_I + 0.467(\pm 2.410) \sigma_R \quad \dots(26)$$

(R = 0.901, n = 9, P > 90%)

$$\delta C_{\beta} (\text{ppm}) = 143.640 (\pm 1.207) - 0.668(\pm 2.366)F + 0.354(\pm 2.189) R \quad \dots(27)$$

(R = 0.977, n = 9, P > 95%)

4. CONCLUSIONS

A series of nine numbers of substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds have been synthesized by condensation of 4-methoxy acetophenone and *ortho* and *meta* substituted benzaldehydes. These synthesized substituted (*E*)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one compounds have been characterized by their physical constants, spectral data. The UV, FT-IR, ¹H and ¹³C NMR spectral data of these has been correlated with Hammett substituent constants and *F* and *R* parameters. From the results of statistical analyses, the effects of substituent on the spectral data have been studied. FT-IR and ¹H and ¹³C NMR spectral correlations produced a greater number of satisfactory correlations. But ¹H NMR spectral data with H_β spectral values gave poor correlations with all Hammett substituents constants and Swain-Lupton's parameters. The UV spectral values and FT-IR CO_{s-trans} few constants only give the satisfactory correlations with Hammett substituents constants and Swain-Lupton's parameters. However, all the multi-regression analyses have shown satisfactory correlations.

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