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Synthesis, structure-parameter correlation and antimicrobial evaluation of 1-(3, 5-dibenzoyloxyphenyl)-3-phenyl-2-propenone compounds

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Abstract

A series of 1-(3,5-dibenzoyloxyphenyl)-3-phenyl-2-propenone compounds are synthesized from 3,5-dibenzoyloxyacetophenone with various substituted benzaldehydes by crossed aldol condensation. The synthesized compounds are characterized by their physical constants and spectral data. Antibacterial and anti-fungal activities of synthesized 1,3-diphenyl-2-propenone compounds are measured by Kirby-Bauer Disc diffusion method.

Keywords: Crossed-Aldol condensation; Boron Trifluoride complex; 1-(3,5-dibenzoyloxyphenyl)-3-phenyl-2-propenone compounds; Substituent effects; Antimicrobial activities.

1. Introduction

Chalcones are 1, 3-diphenyl-2-propenone compounds which available in various flavonoids family plants. In ancient medicine flavonoids family plants are plays an important role in medical field for curing of various diseases. Later researchers found that 1, 3-diphenyl-2-propenone skeletons in the flavonoid family plant extract is reason for various anti-infective activities. Based on that studies various substituted 1, 3-diphenyl-2-propenone compounds synthesised and studied their anti-infective activities [1]. Now a days researchers directed towards to synthesis of this class of compounds is becoming the subject of anti-infective research [2], and many groups have isolated and identified the structures of flavonoids possessing several anti-infective activities [3]. The relationship between flavonoid structure and anti-infective activities are in close agreement has proven by several high-quality investigations [4-6]. Aldol and Crossed-Aldol condensation [7-9] were useful for synthesis of 1,3-diphenyl-2-propenone compounds. Spectral data were useful for prediction of ground state molecular equilibration such as *E s-cis*, *s-trans* and *Z s-cis* and *s-trans* conformers [10].

Chalcones are 1, 3-diphenyl-2-propenones which available in the flavonoids family contains medicinal effect like anti-microbial [11], anti-inflammatory [12], analgesic [13], anti-ulcerative [14], immune-modulatory [15], anti-malarial [16], anti-cancer [17], anti-viral [18], anti-leishmanial [19], anti-oxidant [20], anti-tubercular [21], anti-hyperglycemic [22], anti-oxidant activity [23]. Presence of the reactive keto group and the vinylenic group in the 1, 3-diphenyl-2-propenone compounds and their analogues possesses the antioxidant activity [24]. Compounds that associated with the antioxidant properties are hydroxyl and phenyl group.

Correlation analysis were applied for studying the transition states of reaction mechanism [25], electrochemical redox behaviour [26], qualitative and quantitative analysis [27-29], assessment of substituent effects in oligopeptides [30].

Vanangamudi *et al.* [31] has studied Synthesis, spectral linearity, antimicrobial, antioxidant and insect anti feedant activities of some 2, 5-dimethyl-3-thienyl chalcones. Thirunarayanan *et al.*, [32] has studied the synthesis and spectral correlations of some 1, 3-oxazine-4-thione derivatives and observed satisfactory correlations.

Narender and Popi Reddy [33] had developed a new methodology to synthesize several substituted aryl styryl ketones by using $\text{BF}_3 \cdot \text{Et}_2\text{O}$. The advantages of this method over the existing methods are high yields, simple work-up, short duration, absence of side reactions and easier separation of the products.

With a view to above, there is no report available for UV, IR and NMR spectral correlation analysis with Hammett substituent constants, F and R parameters and antimicrobial activities of 1-(3,5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds. Therefore the authors have taken efforts to study the spectral correlation and antimicrobial activities of the 1-(3,5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds by synthesis and record their UV, IR and NMR spectra.

2. Experimental

2.1 Materials and Methods

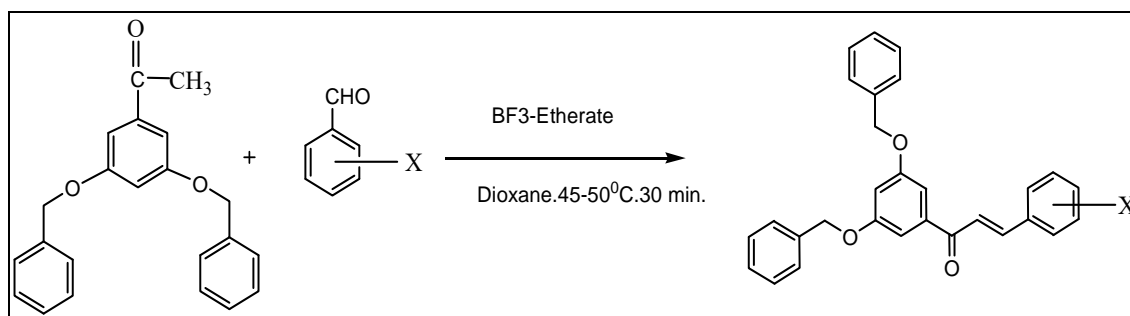
All the chemicals used were purchased from Sigma-Aldrich and E-Merck chemical company. Melting points of all compounds were determined in open glass capillaries on *V-SCIENTIFIC MP-DS* melting point apparatus and are uncorrected. UV spectra measured from *ELICO BL-222 SPECTROMETER*. Infrared spectra (KBr, 4000-400 cm^{-1}) were recorded *SHIMADSU* Fourier transform spectrometer. NMR spectra measured from *INSTRUM AV300* operating at 500MHz for ^1H spectra and 125.46 MHz for ^{13}C spectra in CDCl_3 solvent using TMS as internal standard.

2.2 Synthesis of 1-(3, 5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds

An appropriate equimolar quantity of 3, 5-dibenzyloxy acetophenone (0.01mol) and substituted benzaldehyde (0.01mol) followed by 10 ml of dioxane have been taken in 250 ml flat bottom flask fitted with magnetic stirrer and thermometer. To this mixture 5 g of Borontriluoride-diethyl ether complex catalyst have been added slowly through addition funnel. The mixture have been heated to 45-50 $^\circ\text{C}$ with stirring for 30 minutes [33]. The progress of reaction was monitored with

TLC plate. After completion of reaction the reaction mass poured in to 100 ml of ice water in a 250 ml beaker. The pale yellow precipitate obtained while stirring the mass with teflon rod was washed with cold water and filtered through what man number 40 filter paper and dried.

The obtained pale yellow solid have been recrystallized with ethanol-hexane mixture obtained pale yellow glittering solid. The obtained yield and melting point of all the ten 1,3-diphenyl-2-propenone compounds prepared in this series was presented in table -1.



Scheme-1 Where X = H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH₃, 4-OCH₃, 2-CH₃, 4-CH₃

Fig 1: Synthetic reaction scheme of 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds

Table-1: Physical constants and yield of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

S.NO.	substitution	Molecular Formula	Molecular Weight	Yield %	Melting Point $^\circ\text{C}$
1	H	$\text{C}_{29}\text{H}_{24}\text{O}_3$	420	75	136
2	3-Br	$\text{C}_{29}\text{H}_{23}\text{O}_3\text{Br}$	499	79	179
3	4-Br	$\text{C}_{29}\text{H}_{23}\text{O}_3\text{Br}$	499	81	164
4	2-Cl	$\text{C}_{29}\text{H}_{23}\text{O}_3\text{Cl}$	454.5	76	155
5	3-Cl	$\text{C}_{29}\text{H}_{23}\text{O}_3\text{Cl}$	454.5	80	159
6	4-F	$\text{C}_{29}\text{H}_{23}\text{O}_3\text{F}$	438	89	149
7	2-OCH ₃	$\text{C}_{30}\text{H}_{26}\text{O}_4$	440	68	139
8	4-OCH ₃	$\text{C}_{30}\text{H}_{26}\text{O}_4$	440	76	141
9	2-CH ₃	$\text{C}_{30}\text{H}_{26}\text{O}_3$	424	70	140
10	4-CH ₃	$\text{C}_{30}\text{H}_{26}\text{O}_3$	424	73	143

3. Result and Discussion

3.1 Spectral linearity

In the present investigation the Hammett spectral linearity of these synthesized 1-(3, 5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds has been studied by evaluating the substituent effects on the group frequencies. The assigned spectroscopic data of all 1-(3,5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds such as absorption maximum λ_{max} (nm) of carbonyl groups, infrared carbonyl stretches of $\nu\text{COs-cis}$ and $s\text{-trans}$, the deformation modes of vinyl part CH out of plane, in-plane, CH=CH and $>\text{C}=\text{C}<$ out of planes (cm^{-1}), NMR chemical shifts δ (ppm) of H_α , H_β , C_α , C_β , CO are assigned and these data are correlated with various substituent constants.

3.2 UV spectral study

The absorption maxima (λ_{max} nm) of synthesized 1-(3, 5-dibenzyloxyphenyl)-3-phenyl-2-propenone compounds were measured and presented in Table-2. These absorption maxima (λ_{max} nm) of these compounds were correlated with Hammett substituent constants and F and R parameters using single and multi-linear regression analysis [30-33, 40-45]. 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 λ_0 is the frequency for the parent member of the series. The results of statistical analysis [30-33, 40-45] of these UV absorption maxima (λ_{max} , nm) data with Hammett substituent constants and F and R parameters are presented in Table-3.

3.2.1 Correlation analysis of UV spectral data of 1-(3,5-dibenzoyloxyphenyl)-3-phenyl-2-propenone compounds.

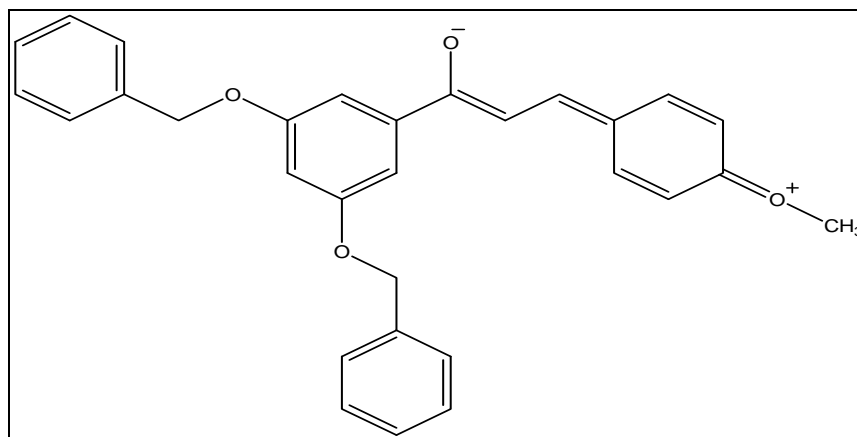
From Table-3, it is evident that the UV absorption maximum $\lambda_{max}(nm)$ values of all the substituted 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown satisfactory correlations except with 2-Cl, 4-F and 2-CH₃ substituents with Hammett substituent constant σ ($r = 0.905$) only. When these substituents that have been given exception when included in regression they reduce the correlation considerably. The UV absorption maximum

$\lambda_{max}(nm)$ values of all the substituted 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlations ($r < 0.900$) with remaining Hammett substituent constants σ^+ , σ_1 & σ_R and F and R parameters.

This is due to the incapability of inductive, field and resonance effects of substituents for predicting the reactivity on the UV absorption maximum $\lambda_{max}(nm)$ values through resonance as per the conjugative structure (1).

Table 2: The ultraviolet absorption maxima (λ_{max} nm), Infrared absorptions (ν cm^{-1}), ¹H-NMR and ¹³C-NMR spectral data of 1-(3,5-dibenzoyloxyphenyl)-3-phenyl-2-propenone compounds.

S. No	Substituents	UV nm	CO s-cis cm^{-1}	CO s-trans cm^{-1}	CH _{ip} cm^{-1}	CH _{op} cm^{-1}	CH=CH _{op} cm^{-1}	C=C _{op} cm^{-1}	H _a (ppm)	H _β (ppm)	δC _a (ppm)	δC _β (ppm)	δCO (ppm)
1	H	312.2	1660.71	1585.49	1165.00	756.10	1024.20	565.14	7.643	7.819	190.00	122.06	130.59
2	3-Br	317.6	1664.57	1591.27	1161.15	740.67	1035.77	549.71	7.579	7.728	189.70	124.85	133.79
3	4-Br	317.0	1662.54	1593.20	1165.00	812.03	1028.06	692.44	7.595	7.751	189.70	122.54	136.43
4	2-Cl	268.0	1670.36	1591.27	1157.29	740.57	1049.26	460.99	7.375	7.470	194.00	127.41	128.65
5	3-Cl	315.0	1680.00	1595.13	1159.22	860.22	1018.22	594.08	7.566	7.743	197.80	127.61	139.08
6	4-F	281.0	1680.00	1598.99	1236.37	837.11	1014.56	609.51	7.482	7.831	190.80	127.55	136.45
7	2-OCH ₃	282.0	1664.57	1587.42	1165.00	748.38	1043.49	526.57	7.607	7.789	190.80	119.37	132.02
8	4-OCH ₃	295.8	1662.64	1593.20	1168.86	734.88	1039.63	580.57	7.785	7.908	189.20	122.44	134.25
9	2-CH ₃	275.0	1593.20	1514.12	1153.42	738.74	1039.63	464.84	7.345	7.428	190.60	128.68	139.04
10	4-CH ₃	290.0	1593.20	1521.84	1168.82	732.95	1041.56	470.63	7.512	7.787	189.20	122.43	134.23



(1)

All the correlations except σ_1 have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to UV absorption maximum $\lambda_{max}(nm)$ values of all the

1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

The single linear plot of σ with UV absorption maximum $\lambda_{max}(nm)$ values is shown in Fig- 2.

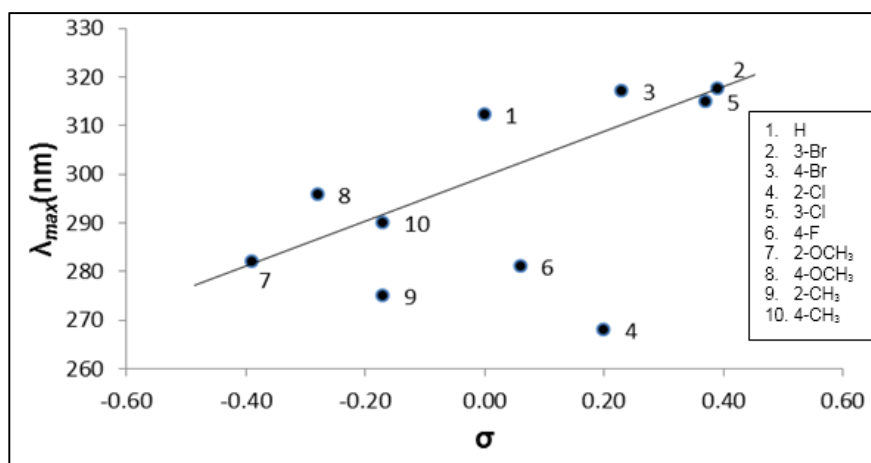


Fig 2: Plot of $\lambda_{max}(nm)$ values of substituted 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds Vs σ

Since most of the single regression analyses have shown poor correlations with Hammett substituent constants σ^+ , σ_1 & σ_R and F and R parameters, it is decided to go for multi regression analysis. The multi regression analysis of the UV absorption maximum λ_{max} (nm) values of all the substituted 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with inductive, resonance and Swain-Lupton's [44] parameters produce satisfactory correlations as shown in equations (2) and (3).

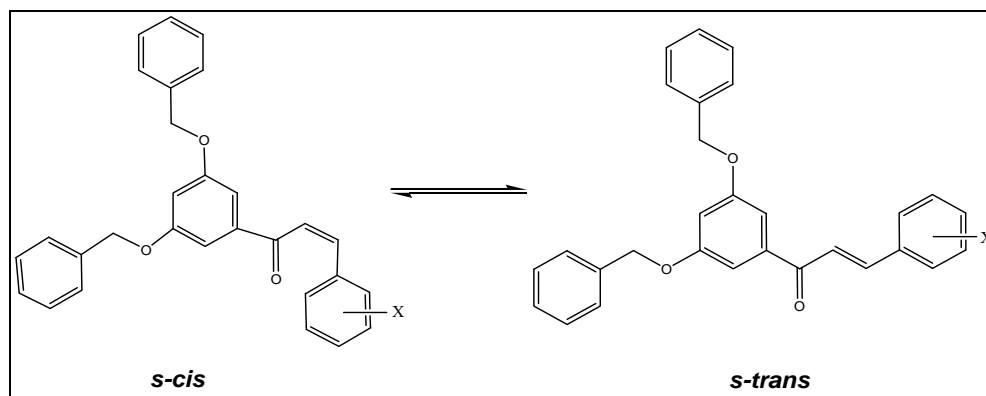
$$UV(\lambda_{max})=301.821(\pm 10.392)+33.204(\pm 27.157)\sigma_1 \\ 65.019(\pm 33.376)\sigma_R \quad \dots (2)$$

$$UV(\lambda_{max})=302.536(\pm 11.318)+28.498(\pm 30.654)F+ \\ 54.264(\pm 36.352)R \quad \dots (3)$$

(R = 0.944, n = 10, P > 95%)

3.3. IR spectral study

The stretching frequencies for carbonyl absorption are assigned based on the assignments made by Hays and Timmons [45] for *s-cis* and *s-trans* conformers at 1690 and 1670 cm^{-1} , respectively. These data have been correlated with



(2)

From Table-3, it is evident that the infrared frequency $\nu_{C=O_{s-cis}}$ (cm^{-1}) values of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown satisfactory

Hammett substituent constants and Swain-Lupton's constants [44] and are presented in Table-3. In this correlation the structure parameter Hammett equation employed is as shown in the following equation:

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

where ν is the carbonyl frequencies of substituted system and ν_0 is the corresponding quantity of unsubstituted system, σ is a Hammett substituent constant, which in principle is characteristics of the substituent and ρ is a reaction constant which is depend upon the nature of the reaction.

3.3.1 Correlation analysis of IR spectral data of 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

The assigned $\nu_{CO}(\text{cm}^{-1})$ stretches of the *s-cis* and *s-trans* conformers and $\nu_{CH_{ip}}$, $\nu_{CH_{op}}$, $\nu_{CH=CH_{op}}$ and $\nu_{C=C_{op}}(\text{cm}^{-1})$ deformation modes of all the substituted 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds in series-C are presented in Table-2 and the corresponding *s-cis* and *s-trans* conformers are shown in (2).

correlations except those with 2- CH_3 and 4- CH_3 substituents with Hammett substituent constants σ_1 ($r = 0.901$) and F ($r = 0.907$) parameter.

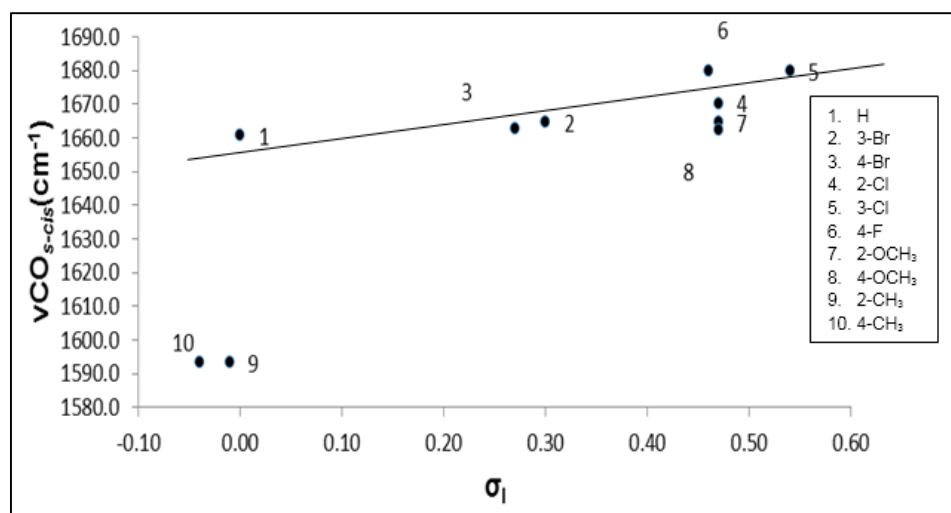


Fig-3: Plot of $\nu_{CO_{s-cis}}$ (cm^{-1}) values of substituted 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds Vs σ_1

Infrared stretching frequency $\nu_{CO_{s-trans}}(\text{cm}^{-1})$ values of the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 2- CH_3 and 4- CH_3 substituents

have shown satisfactory correlations with Hammett substituent constants σ_1 ($r = 0.900$) and F ($r = 0.907$) parameter.

Infrared frequency $\nu\text{CH}_{ip}(\text{cm}^{-1})$ values of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds, except that with 4-F substituent have shown satisfactory correlation with F ($r = 0.900$) and R ($r = 0.905$) parameters.

Infrared frequency $\nu\text{CH}_{op}(\text{cm}^{-1})$ values of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 4-Br, 3-Cl and 4-F substituents have shown satisfactory correlation with Hammett substituent constants σ ($r = 0.960$), σ^+ ($r = 0.904$), σ_I ($r = 0.900$) and F ($r = 0.906$) parameter.

Infrared frequency $\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1})$ values of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds

have shown poor ($r < 0.900$) correlations with all the Hammett substituent constants namely σ , σ^+ , σ_I and σ_R and F and R parameters.

Infrared frequency $\nu\text{C}=\text{C}_{op}(\text{cm}^{-1})$ values of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds, except those with 4-Br and 2-Cl substituents have shown satisfactory correlations with Hammett substituent constants σ_I ($r = 0.905$) and R ($r = 0.900$) parameter.

When these substituents that have been given exception are included in regression they reduce the correlations considerably.

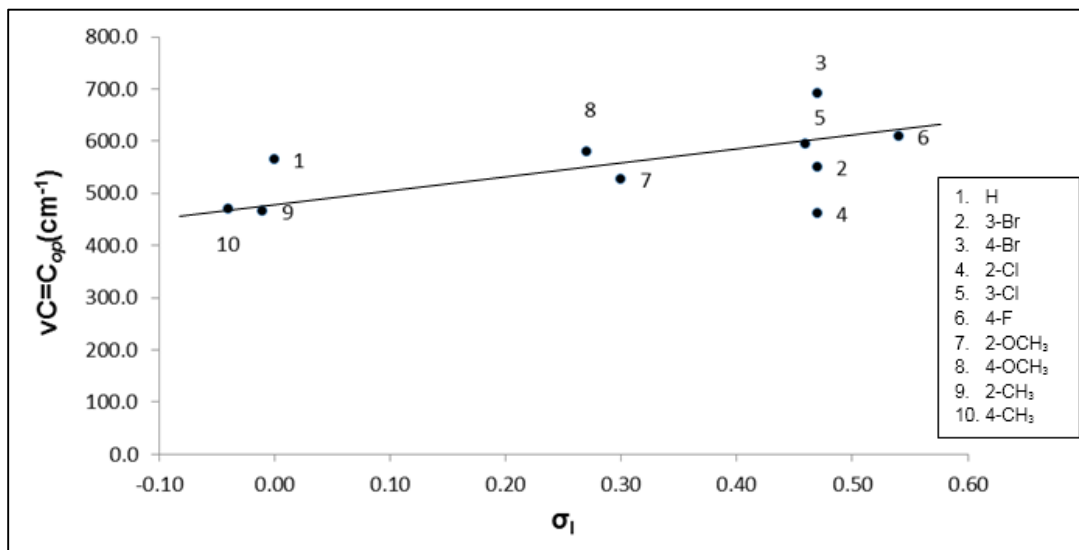


Fig-4: Plot of $\nu\text{C}=\text{C}_{op}(\text{cm}^{-1})$ values of substituted 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds Vs σ_I

The poor correlations of ($r < 0.900$) with remaining Hammett substituent constants and F and R parameters is attributed to the weak polar and resonance effects of the substituents for predicting the reactivity on the infrared frequency through resonance as per the conjugative structure (1).

In this correlations the negative ρ values indicates the operation of reverse substituent effect and the positive ρ values indicates the operation of normal substituent effect with respect to Hammett substituent constants and Swain-Lupton's ^[44] constants.

In this case some of the single regression analyses have shown poor correlations with Hammett constant and F and R parameter. So, it is decided to go for multi regression analysis. The multi regression analysis of all the infrared values of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds with inductive, resonance and Swain-Lupton's ^[44] parameters have shown satisfactory correlations as shown in equations (5) - (16).

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1})=1618.748(\pm 13.256)+111.126(\pm 34.640)\sigma_I-7.515(\pm 42.573)\sigma_R \quad \dots (5)$$

($R = 0.980$, $n = 10$, $P > 95\%$)

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1})=1624.899(\pm 14.704)+107.58(\pm 39.823)F+16.515(\pm 47.225)R \quad \dots (6)$$

($R = 0.975$, $n = 10$, $P > 95\%$)

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1})=1544.645(\pm 13.421)+106.129(\pm 35.072)\sigma_I-5.786(\pm 43.104)\sigma_R \quad \dots (7)$$

($R = 0.978$, $n = 10$, $P > 95\%$)

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1})=1549.907(\pm 14.906)+99.651(\pm 40.372)F+11.586(\pm 47.876)R \quad \dots (8)$$

($R = 0.972$, $n = 10$, $P > 95\%$)

$$\nu\text{CH}_{ip}(\text{cm}^{-1})=1133.31(\pm 17.133)-22.305(\pm 32.757)\sigma_I-29.183(\pm 25.615)\sigma_R \quad \dots (9)$$

($R = 0.951$, $n = 9$, $P > 95\%$)

$$\nu\text{CH}_{ip}(\text{cm}^{-1})=1132.24(\pm 14.962)-21.422(\pm 28.962)F-29.822(\pm 24.577)R \quad \dots (10)$$

($R = 0.949$, $n = 9$, $P > 90\%$)

$$\nu\text{CH}_{op}(\text{cm}^{-1})=824.169(\pm 5.134)-3.271(\pm 9.816)\sigma_I-1.452(\pm 7.676)\sigma_R \quad \dots (11)$$

($R = 0.958$, $n = 9$, $P > 95\%$)

$$\nu\text{CH}_{op}(\text{cm}^{-1})=822.990(\pm 4.455)-0.929(\pm 8.623)F-2.022(\pm 7.317)R \quad \dots (12)$$

($R = 0.967$, $n = 9$, $P > 95\%$)

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1})=1021.80(\pm 4.007)-3.904(\pm 7.756)F-2.629(\pm 6.582)R \quad \dots (13)$$

($R = 0.949$, $n = 9$, $P > 90\%$)

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1})=1023.38(\pm 4.540)-6.781(\pm 8.680)\sigma_I-1.119(\pm 6.788)\sigma_R \quad \dots (14)$$

($R = 0.938$, $n = 9$, $P > 90\%$)

$$\nu\text{C}=\text{C}_{op}(\text{cm}^{-1})=569.046(\pm 20.073)-51.226(\pm 38.378)\sigma_I+59.210(\pm 30.011)\sigma_R \quad \dots (15)$$

($R = 0.955$, $n = 9$, $P > 95\%$)

$$\nu\text{C}=\text{C}_{op}(\text{cm}^{-1})=573.692(\pm 12.846)-58.862(\pm 24.867)F+57.517(\pm 21.102)R \quad \dots (16)$$

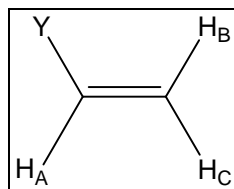
($R = 0.954$, $n = 9$, $P > 95\%$)

Table 3: Results of statistical analysis of UV, IR spectral values of 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds with Hammett σ , σ^+ , σ_I , σ_R constants and F and R parameters.

Absorption	Constants	R	I	ρ	s	n	Correlated derivatives
$\lambda_{max}(nm)$	σ	0.905	322.98	-4.997	8.84	7	H, 3-Br, 4-Br, 3-Cl, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃
	σ^+	0.804	322.5	-4.597	8.74	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.715	318.88	10.222	8.7	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.847	318.35	-18.421	7.15	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.704	317.74	12.418	8.46	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.833	317.64	-17.639	6.99	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
Frequency	constant	r	I	ρ	s	n	Correlated derivatives
$\nu_{CO_{s-cis}}(cm^{-1})$	σ	0.754	1654.16	22.108	12.39	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.872	1656.28	15.57	13.05	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.901	1641.51	41.785	11.24	8	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃
	σ_R	0.832	1661.48	23.006	13.94	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.907	1653.01	34.701	12.49	8	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃
	R	0.833	1661.77	19.893	14.16	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\nu_{CO_{s-trans}}(cm^{-1})$	σ	0.805	1598.41	7.587	5.88	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.798	1599.14	5.285	5.77	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.900	1593.59	15.684	5.02	8	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃
	σ_R	0.834	1599.44	1.326	6.44	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.907	1592.82	16.517	4.68	8	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃
	R	0.763	1599.51	1.316	6.44	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\nu_{CH_{ip}}(cm^{-1})$	σ	0.705	1183.67	-13.44	33.25	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.514	1182.37	-6.780	33.54	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.685	1207.16	-70.05	28.44	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.842	1184.18	8.060	33.65	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.900	1208.51	-68.27	28.28	9	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.905	1185.69	12.09	33.51	9	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\nu_{CH_{op}}(cm^{-1})$	σ	0.960	860.77	-33.92	30.23	7	H, 3-Br, 2-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.904	857.50	-22.71	31.15	7	H, 3-Br, 2-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.900	869.66	-34.40	32.35	7	H, 3-Br, 2-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.807	848.78	-38.65	31.42	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.906	875.71	-47.58	31.01	7	H, 3-Br, 2-Cl, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.811	849.21	-30.08	32.06	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\nu_{CH=CH_{op}}(cm^{-1})$	σ	0.847	1070.64	4.14	29.54	8	H, 4-Br, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.827	1071.05	-4.20	29.5	8	H, 4-Br, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.828	1076.28	-14.78	29.35	8	H, 4-Br, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.819	1071.85	3.58	29.57	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.840	1069.28	4.59	29.57	9	H, 3-Br, 4-Br, 2-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.802	1070.44	-2.17	29.59	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\nu_{C=C_{op}}(cm^{-1})$	σ	0.762	565.48	-44.83	35.9	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.722	561.18	-38.06	34.95	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.905	600.35	-110.78	28.89	8	H, 3-Br, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.806	554.91	-27.66	39.86	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.900	597.84	-95.82	31.5	8	H, 3-Br, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.714	552.54	-31.26	39.41	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃

3.4.1 ¹H NMR spectral study

From the ¹H NMR spectra of synthesized 1-(3, 5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds, the signals of the ethylenic protons have been assigned. The chemical shifts of H_α are higher field than those of H_β in the present investigated. The β proton doublet in most cases is well separated from aromatic protons.



(3)

Solcaniova and Toma [46] have investigated the effect of substituent on the ¹H NMR Spectra of 1, 3-diphenyl-2-propenone compounds observed. In their investigation H_α chemical shift are more sensitive to the effects of substituents.

Further Solcaniova and Toma [46] observed opposite sign of the slopes for H_α and H_β in their correlations of chemical shift with substituent constants (3). This was attributed by them to the polarization of the C=O double bond being predominantly caused by the carbonyl group.

The chemical shifts values, δH_{α} (ppm) and δH_{β} (ppm) of all the 1-(3,5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds have been correlated with Hammett substituent constants and F and R parameters using single and multi-regression analyses.

The Hammett equation employed is as shown in equation (17)

$$\delta = \rho\sigma + \delta_0 \dots \quad (17)$$

Where δ_0 is the ¹H NMR chemical shift of the corresponding parent compound.

The assigned ¹H NMR data of δH_{α} and δH_{β} of all the 1-(3, 5-dibenzoyloxyphenyl)-3-phenylprop-2-en-1-one compounds in the present investigation are presented in Table-2. These values were correlated with Hammett substituent constants and F and R parameters. The results of statistical analysis are given in Table-4.

Table 4: The results of statistical analysis of ^1H NMR chemical shift $\delta\text{H}_\alpha(\text{ppm})$ and $\delta\text{H}_\beta(\text{ppm})$ values of Substituted 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with Hammett constants σ , σ^+ , σ_I & σ_R and F and R parameters.

Chemical shift	Constants	r	I	ρ	s	n	Correlated derivatives
$\delta\text{H}_\alpha(\text{ppm})$	σ	0.719	7.109	0.174	0.1	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.831	7.126	0.129	0.102	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.702	7.076	0.142	0.119	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.715	7.164	0.165	0.114	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.625	7.059	0.132	0.12	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.821	7.169	0.155	0.114	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
$\delta\text{H}_\beta(\text{ppm})$	σ	0.814	7.513	0.085	0.145	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.834	7.522	0.049	0.147	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.712	7.436	0.243	0.135	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.729	7.504	-0.079	0.147	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.722	7.422	0.26	0.132	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	R	0.741	7.499	-0.082	0.147	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃

r = correlation co-efficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents

3.4.1 Correlation analysis of ^1H NMR spectral data of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

From Table-4 it is evident that the ^1H NMR chemical shift δH_α (ppm) values of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with all the substituents have shown poor correlations ($r < 0.900$) with Hammett substituent constants and F and R parameter.

The ^1H NMR chemical shift δH_β (ppm) values of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with all the substituents have shown poor correlations ($r < 0.900$) with Hammett substituent constants and F and R parameter.

This is attributed to the weak inductive and field effects of the substituents for predicting the reactivity on the ^1H NMR chemical shift through resonance as per the conjugative structure (1).

Most of the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to the ^1H NMR chemical shift values of all the (*E*)-1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

In this case all the single regression analyses have shown poor correlations with Hammett constant and F and R parameter. So, it is decided to go for multi regression analysis.

The multi regression analysis of the ^1H NMR chemical shift values of all the (*E*)-1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with inductive, resonance and Swain-Lupton's $^{[32]}$ parameters produce satisfactory correlations as shown in equations (18) - (21).

$$\delta\text{H}_\alpha(\text{ppm}) = 7.519(\pm 0.087) - 0.026(\pm 0.229)\sigma_I - 0.122(\pm 0.281)\sigma_R \quad \dots(18)$$

$$(R = 0.947, n = 10, P > 90\%)$$

$$\delta\text{H}_\alpha(\text{ppm}) = 7.506(\pm 0.080) - 0.105(\pm 0.228)F - 0.229(\pm 0.271)R \quad \dots(19)$$

$$(R = 0.961, n = 10, P > 95\%)$$

$$\delta\text{H}_\beta(\text{ppm}) = 7.664(\pm 0.102) + 0.002(\pm 0.268)\sigma_I - 0.217(\pm 0.329)\sigma_R \quad \dots(20)$$

$$(R = 0.975, n = 10, P > 95\%)$$

$$\delta\text{H}_\beta(\text{ppm}) = 7.633(\pm 0.097) - 0.008(\pm 0.264)F - 0.300(\pm 0.314)R \quad \dots(21)$$

$$(R = 0.988, n = 10, P > 95\%)$$

3.5. ^{13}C NMR spectral study

Scientists and physical organic chemists $^{[10, 11, 35-38, 45-50]}$, have made extensive study of ^{13}C NMR spectra for a large number of different ketones and styrenes. The assigned vinyl C_α , C_β and carbonyl carbon chemical shifts of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds are presented in Table-2. These values were correlated with

Hammett substituent constants and F and R parameters. The results of statistical analysis are given in Table-5.

3.5.1 Correlation analysis of ^{13}C NMR spectral data of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

From Table-5, it is evident that the δC_α chemical shifts (ppm) values of the

1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlations ($r < 0.900$) with all the Hammett substituent constants and F and R parameters.

The δC_α chemical shifts (ppm) values of the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlations ($r < 0.900$) with all the Hammett substituent constants and F and R parameters.

The δC_β chemical shifts (ppm) values of the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlations ($r < 0.900$) with all the Hammett substituent constants namely σ , σ^+ , σ_I , σ_R and F and R parameters.

This is due to the incapability of polar, inductive, field and resonance effects of the substituents for predicting the reactivity on the ^{13}C NMR chemical shift through resonance as per the conjugative structure (1).

Most of the correlations have shown negative ρ values with all the Hammett substituent constants and F and R parameter. It indicates that the reverse substituent effect operates with respect to ^{13}C NMR chemical shift values of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds. In this case all the single regression analyses have shown poor correlations with all the Hammett substituent constants and F and R parameters. So, it is decided to go for multi regression analysis.

The multi regression analysis of the ^{13}C NMR chemical shift values of all the 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with inductive, resonance and Swain-Lupton's $^{[44]}$ parameters produce satisfactory correlations as shown in equations (22) - (27).

$$\delta\text{C}_\alpha(\text{ppm}) = 190.281(\pm 1.685) + 5.625(\pm 4.403)\sigma_I + 3.073(\pm 5.412)\sigma_R \quad \dots(22)$$

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

$$\delta\text{C}_\alpha(\text{ppm}) = 191.089(\pm 1.668) + 5.662(\pm 4.517)F + 5.695(\pm 5.357)R \quad \dots(23)$$

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

$$\delta\text{C}_\alpha(\text{ppm}) = 124.326(\pm 62.101) + 5.350(\pm 5.231)\sigma_I + 5.622(\pm 6.429)\sigma_R \quad \dots(24)$$

$$(R = 0.903, n = 10, P > 95\%)$$

$$\delta\text{C}_\alpha(\text{ppm}) = 124.368(\pm 1.912) + 7.020(\pm 5.179)F + 6.926(\pm 6.142)R \quad \dots(25)$$

$$(R = 0.904, n = 10, P > 95\%)$$

$$\delta C_{\beta}(\text{ppm}) = 134.494(\pm 2.353) + 1.041(\pm 6.155)\sigma_I + 1.393(\pm 7.565)\sigma_R \quad \dots(26)$$

(R = 0.907, n = 10, P > 90%)

$$\delta C_{\beta}(\text{ppm}) = 133.981(\pm 2.341) + 1.716(\pm 6.342)F + 0.195(\pm 7.521)R \quad \dots(27)$$

(R = 0.901, n = 10, P > 90%)

Table 5: The results of statistical analysis of ^{13}C NMR chemical shift $\delta\text{CO}(\text{ppm})$, $\delta\text{C}_{\alpha}(\text{ppm})$ and $\delta\text{C}_{\beta}(\text{ppm})$ values of substituted 1- (3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds with Hammett constants σ , σ^+ , σ_I & σ_R and F and R parameters.

Chemical Shift	Constants	r	I	ρ	s	n	Correlated derivatives
$\delta\text{CO}(\text{ppm})$	σ	0.847	191.75	-1.683	2.144	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.849	191.59	-0.932	2.203	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.849	193.65	-5.819	1.685	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.709	191.64	-0.212	2.261	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.802	193.68	-5.465	1.716	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
R	0.715	191.71	0.435	2.581	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃	
$\delta\text{C}_{\alpha}(\text{ppm})$	σ	0.849	119.80	0.422	3.314	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.843	119.84	0.392	3.312	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.725	118.79	2.953	3.229	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.717	119.55	1.288	3.295	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.729	119.27	1.478	3.295	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
R	0.715	119.82	0.087	3.319	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃	
$\delta\text{C}_{\beta}(\text{ppm})$	σ	0.712	141.91	-1.416	3.051	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ^+	0.710	141.77	-0.850	3.075	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_I	0.703	141.96	-0.538	3.108	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	σ_R	0.705	141.22	-2.473	3.018	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
	F	0.711	142.38	-1.588	3.081	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃
R	0.805	141.48	-1.048	3.091	10	H, 3-Br, 4-Br, 2-Cl, 3-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 2-CH ₃ , 4-CH ₃	

r = correlation co-efficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents

4. Antimicrobial Activity

4.1 Antibacterial activity:

The newly synthesized 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds (1-9) were subjected to antibacterial activity against gram positive bacteria *Bacillus subtilis*, *M. luteus* and *S.aureus* gram negative bacteria *Escherichia coli*, *P. aeruginosa* and *k. pneumonias* by using Kirby Bauer [47]. disc diffusion method. The agar medium was purchased from *HI MEDIA* Laboratories Ltd, Mumbai, India. The agar medium prepared by dissolving 2.5 g of agar in 100 ml water at boiled condition as per standard procedure. The bubble free medium poured in to Petri dishes and allowed to cool under closed condition for gel formation. After streaking microorganism what man no-40 discs of 6.0 mm in diameter laid on the gel to identify the inhibition zones. The test compounds prepared by dissolving 10 mg each compound in 5 ml of dimethyl sulphoxide. The solution of each compound 0.1 ml were added on what man disc and incubated at 37°C for 24 Hour.

A reference standard drug of gram positive and gram negative bacteria was made by dissolving 10.0 mg of ampicillin in 5.0 ml of distilled water separately. All the experiments were carried out duplicate to avoid error. Simultaneously reference were tested with 0.1 ml of dimethyl sulphoxide which not reveal any zone of inhibition. Diameter of inhibition zone produced by each compound was measured in mm. The results are given in Table-6.

4.1.1 Antibacterial activity against *Bacillus subtilis*

Analysis of the zone of inhibition (mm) values reveals that only one compound with 2-OCH₃ substituent has shown good antibacterial activity and the five compounds with 3-Br, 3-Cl, 4-F and 4-OCH₃, substituted has shown moderate antibacterial activity. The remaining four compounds with H (parent), 4-Br, 2-Cl and 2-CH₃ substituents in have shown poor antibacterial activity.

4.1.2 Antibacterial activity against *Micrococcus luteus*.

Analysis of the zone of inhibition (mm) values reveals that two compounds with 4-Br and 2-Cl substituents has shown good

antibacterial activity and four compounds with 4-F, 2-OCH₃, 4-OCH₃ and 2-CH₃ substituents has shown moderate antibacterial activity.

The remaining three compounds with H (parent), 3-Br, and 3-Cl substituents has shown poor antibacterial activity.

4.1.3 Antibacterial activity against *Staphylococcus aureus*

The eight compounds with H (parent), 3-Br, 4-Br, 2-Cl, 3-Cl, 2-OCH₃, 4-OCH₃ and 2-CH₃ substituents has shown moderate antibacterial activity. The only one with 4-F substituent has shown poor antibacterial activity.

4.1.4 Antibacterial activity against *Escherichia coli*

Analysis of the zone of inhibition (mm) values reveals that two compounds with 4-Br and 4-F substituents has shown good antibacterial activity and five compounds with H (parent), 3-Br, 2-Cl, 4-OCH₃ and 2-CH₃ substituents has shown moderate antibacterial activity.

The remaining two compounds with 3-Cl, and 2-OCH₃ substituents has shown poor antibacterial activity.

4.1.5 Antibacterial activity against *Pseudomonas aeruginosa*

Analysis of the zone of inhibition (mm) values reveals that three compounds with 2-Cl, 2-CH₃ and 4-F substituents has shown good antibacterial activity and three compounds with 4-Br, 3-Cl, and 2-OCH₃, substituents has shown moderate antibacterial activity.

The remaining three compounds with H (parent), 3-Br and 4-OCH₃ substituents has shown poor antibacterial activity.

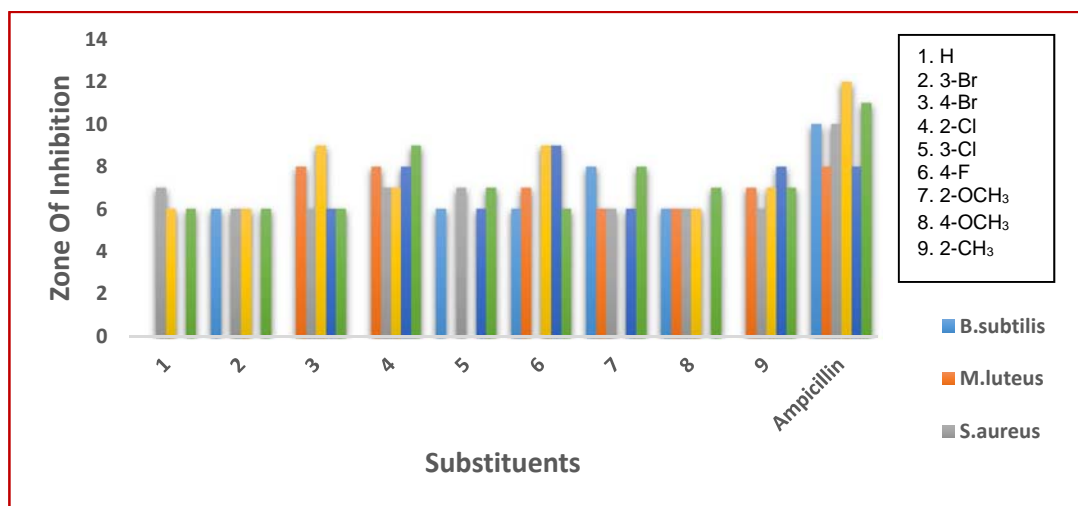
4.1.6 Antibacterial activity against *Klebsiella pneumoniae*

Analysis of the zone of inhibition (mm) values reveals that two compounds with 2-Cl and 2-OCH₃ substituents has shown good antibacterial activity. The remaining seven compounds with H (parent), 3-Br, 4-Br, 3-Cl, 4-F, 4-OCH₃ and 2-CH₃ substituents has shown moderate antibacterial activity.

Table 6: Antibacterial activity of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

S. No	Substituents	Zone of Inhibition (mm)					
		Gram positive Bacteria			Gram negative Bacteria		
		<i>B.subtilis</i>	<i>M. luteus</i>	<i>S.aureus</i>	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>k. pneumonias</i>
1	H	0	0	7	6	0	6
2	3-Br	6	0	6	6	0	6
3	4-Br	0	8	6	9	6	6
4	2-Cl	0	8	7	7	8	9
5	3-Cl	6	0	7	0	6	7
6	4-F	6	7	0	9	9	6
7	2-OCH ₃	8	6	6	0	6	8
8	4-OCH ₃	6	6	6	6	0	7
9	2-CH ₃	0	7	6	7	8	7
Standard	Ampicillin	10	8	10	12	8	11
control	DMSO	0	0	0	0	0	0

(-) Indicates no zone of inhibition formed

**Fig 5:** Clustered chart of antibacterial activity of substituted 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

4.2 Antifungal Activity

The antifungal effect of the substituted of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds using potato-dextrose-agar (PDA) medium same cup and plate method against *Aspergillus niger*, *Trichoderma viride* and *Mucor species*. Preparation of nutrient broths subculture base layer medium and PDA-medium was done as per the standard procedure. A reference standard drug fluconazole 10 mg dissolved in 5ml of water 0.1 ml of solution used as a control which did not reveal any inhibition. The experiments were duplicated to minimize the error. Diameter of inhibition zone produced by each compound was measured in mm and tabulated in table- 7.

4.2.1 Antifungal activity against *Aspergillus niger*

Analysis of the Zone of inhibition (mm) values reveals that the two compounds with 3-Cl and 2-OCH₃ substituent has shown good antifungal activity. The remaining seven compounds with H (parent), 3-Br, 4-Br, 2-Cl, 4-F, 4-OCH₃ and 2-CH₃ substituents in series-C has shown moderate antifungal activity.

4.2.2 Antifungal activity *Trichoderma viride*

Analysis of the Zone of inhibition (mm) values reveals that the two compounds with 4-F and 2-OCH₃ substituents has shown good antifungal activity and the four compounds with 3-Br, 2-Cl, 4-OCH₃ and 2-CH₃ substituents has shown moderate antifungal activity. The remaining three compounds with H

(parent), 4-Br and 3-Cl substituents has shown poor antifungal activity.

4.2.3 Antifungal activity *Mucor Species*

Analysis of the Zone of inhibition (mm) values reveals that the only two compounds with 4-Br and 2-OCH₃ substituents has shown good antifungal activity and six compounds with H (parent), 2-Cl, 3-Cl, 4-F, 4-OCH₃ and 2-CH₃ substituents has shown moderate antifungal activity. The remaining one compound with 3-Br substituent has shown poor antifungal activity.

Table 7: Antifungal activity of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

S. No	Substitution	Mean zone of inhibition (mm)		
		<i>A. Niger</i>	<i>T. Viride</i>	<i>M. Species</i>
1	H	7	0	6
2	3-Br	6	6	0
3	4-Br	6	0	8
4	2-Cl	6	6	6
5	3-Cl	8	0	6
6	4-F	6	8	7
7	2-OCH ₃	9	8	8
8	4-OCH ₃	6	6	7
9	2-CH ₃	7	6	6
Control	DMSO	0	0	0
Standard	Fluconazole	12	11	12

(-) Indicates no zone of inhibition formed.

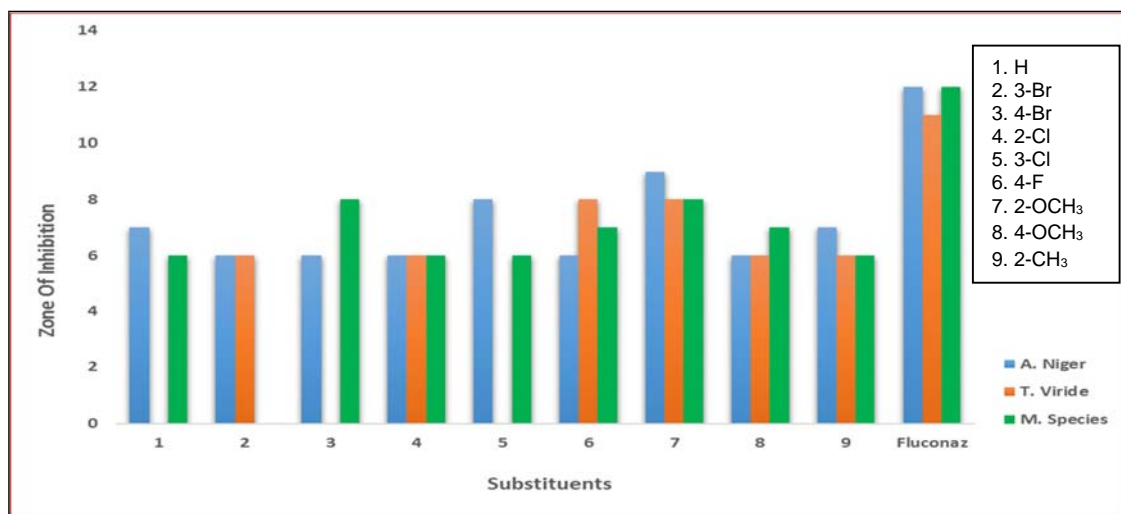


Fig 6: Clustered chart of antifungal activity of substituted 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds.

5. Conclusion

Some of 1-(3,5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have been synthesized by condensation of 3,5-dibenzyloxyacetophenone and substituted benzaldehydes in the presence of boron trifluoride-diethyl ether complex catalyst. This reaction protocol offers a simple, easier work-up procedure and good yields. The 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have been characterized by their physical constants, spectral data.

The UV, IR, NMR spectral data of these 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds has been correlated with Hammett substituent constants, *F* and *R* parameters. From the results of statistical analysis the effects of substituent on the spectral data have been studied.

The antimicrobial activities of all synthesized 1-(3, 5-dibenzyloxyphenyl)-3-phenylprop-2-en-1-one compounds have been studied using Kirby-Bauer disc diffusion method. The screening results revealed that most of the compounds shown good antibacterial activity and moderate antifungal activities.

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