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SYNTHESIS, STRUCTURE-PARAMETER CORRELATION AND ANTIMICROBIAL EVOLUATION OF 1-(4-ISOBUTYLPHENYL)-3-PHENYL-2-PROPENONE COMPOUNDS

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Abstract: **A series of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds are synthesized from 4-isobutyl acetophenone 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-(4-isobutylphenyl)-3-phenyl-2-propenone compounds are measured by Kirby-Bauer disc diffusion method. The bacterial strains used are gram positive bacteria Bacillus subtilis, M.luteus and S.aureus gram negative bacteria Escherichia coli, P.aeruginosa and k.pneumonia and anti-fungal studies with Aspergillus niger, Tricoderma viride and Mucor species.**

Keywords: **Crossed-Aldol condensation; Thionyl chloride /Ethanol; 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds; Substituent effects; Antimicrobial activities.**

1. INTRODUCTION

In ancient medical treatments herbal plants are plays an important role for curing of many diseases. Over a period of time researchers found out the structure of core drug ingredients present in the plant which curing of particular disease. A tremendous changes in medical and bulk drug manufacturing field occurs after identification structure of core ingredients. The core important of this types researches is helping to produce new drugs with enhance activity, reducing side effect and met the medicinal need according to population growth.

In this series researchers found out that flavonoids and isoflavonoids are widely present in edible plants consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β-unsaturated carbonyl system[1]. Among the flavonoids, chalcones are an interesting target class of compounds which are extensively investigated due to their broad spectrum of biological activities[2]. Chalcones are 1, 3 diaryl-2-propenones compounds which synthasised by crossed aldol condensation method.[3-5] 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[6].

Chalcones are 1, 3 diaryl-2-propenones compounds which contains medicinal effect like anti-microbial[7-8], anti-inflammatory[9], analgesic[10], anti-ulcerative[11], immune-modulatory[12], anti-malarial[13], anti-cancer[14], anti-viral[15], anti-leishmanial[16], anti-oxidant[17], anti-tubercular[18], anti-hyperglycemic[19]. A compound having anti-oxidant activity prevents and counteracts the damage of the human tissue by the normal effects of physiological oxidation[20] etc. Presence of the reactive keto group and the vinylenic group in the chalcones and their analogues possesses the antioxidant activity[21].

The correlation analysis were applied for studying the transition states of reaction mechanism[22-23], electro chemical redox behaviour[24], qualitative and quantitative analysis[25-26], assessment of substituent effects in oligopeptides[27].

Hasan *et.al.*,[28] had synthesized a new fluorinated aryl styryl ketone namely (E)-3-(4-fluorophenyl)-1-(4-hydroxylphenyl)prop-2-en-1-one by Claisen Schmidt condensation using thionyl chloride- Ethanol as catalyst. The structure of the synthesized compound has been characterized by TLC, melting point, UV, and IR Spectroscopy, and elemental microanalysis.

Vanangamudi *et.al.*,[30] had synthesized series of substituted styryl 3, 5-dichloro-2-hydroxyphenyl ketones had been synthesized using thionyl chloride-ethanol by crossed-aldol condensation method. The yield of aryl styryl ketones were more than 80%. The synthesized aryl styryl ketones were characterized by analytical and spectroscopic data. Therefore the authors have taken efforts to study the spectral correlation and antimicrobial activities[31] of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds by synthesis and record their UV, IR and NMR spectra.

2. EXPERIMENTAL

2.1 Materials and Methods

2.1.1 Instrumentation for UV spectra

The UV spectra of all the 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds under investigation were recorded using *ELICO BL-222 SPECTROMETER* (λ_{max}) in spectral grade Methanol at CAS in Marine Biology, Annamalai University, Portonovo.

2.1.2 Instrumentation for IR spectra

The IR spectra of all the nine compounds under investigation were recorded using SHIMADZU FT-IR spectrophotometer at CAS in Marine Biology, Annamalai University, Portonovo.

2.1.3 Instrumentation for ^{1}H and ^{13}C NMR spectra

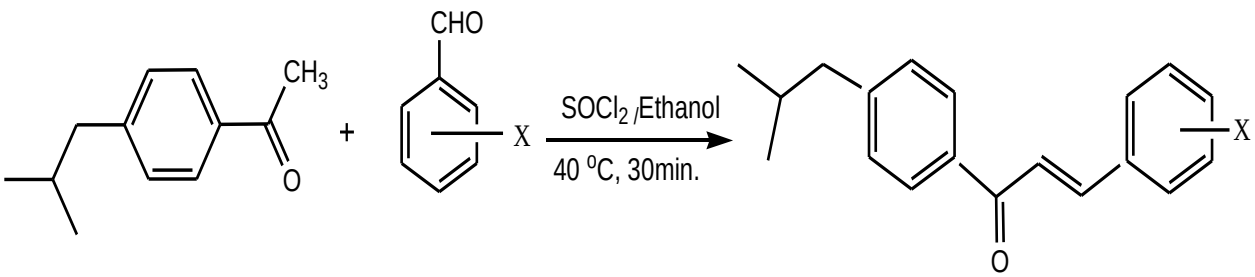
NMR spectra measured from *INSTRUM AV300* operating at 500MHz for ^{1}H spectra and 125.46 MHz for ^{13}C spectra in $CDCl_3$ solvent using TMS as internal standard from INDIAN INSTITUTE OF TECHNOLOGY, CHENNAI.

All chemicals used were purchased from Sigma-Aldrich and E-Merck chemical company. The reaction carried out in round bottom flask fitted with stirrer and thermometer. Melting points of all chalcones were determined in open glass capillaries on *V-SCIENTIFIC MP-DS* melting point apparatus and are uncorrected.

2.2 Synthesis of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds

An appropriate equimolar quantities of 0.01 mole of 4-isobutylacetophenone and 0.01 mole of substituted benzaldehyde and mixed with 5g of thionyl chloride in 20 ml of ethanol. This mixture stirring well in 30 min and slowly raise the temperature to 40 °C. The completion of reaction was tested by TLC method.

After completion of reaction[28-30] the mass poured in to 100 g of ice water the pale yellow precipitate obtained was recrystallised with ethanol n-hexane. A pale yellowish green glittering solid obtained. Melting points and yield of all the nine substituted 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds synthasised in this series was tabulated in **table-1**



Where X = H, 3 -Br, 4-Br, 3-Cl, 4 -Cl, 4 -F, 2 -OCH_3, 4 -CH_3, 3 -NO_2

Fig-1. Synthetic reaction scheme of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

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Table-1: Physical constants and yield data of substituted 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

S.No	Substitution	Molecular Formula	Molecular Weight	Yield %	Melting Point ^{0}C
1	H	$C_{19}H_{20}O$	264	83	96
2	3-Br	$C_{19}H_{19}OBr$	343	85	126
3	4-Br	$C_{19}H_{19}OBr$	343	85	122
4	3-Cl	$C_{19}H_{19}OCl$	298.5	80	119
5	4-Cl	$C_{19}H_{19}OCl$	298.5	80	116
6	4-F	$C_{19}H_{19}OF$	282	78	109
7	2-OCH_3	$C_{19}H_{22}O_2$	294	76	110
8	4-CH_3	$C_{19}H_{22}O$	278	76	105
9	3-NO_2	$C_{19}H_{19}NO_3$	309	79	134

3. RESULT AND DISCUSSION

3.1 Spectral linearity

In the present investigation the Hammett spectral linearity of these synthesized1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds has been studied by evaluating the substituent effects on the group frequencies. The assigned spectroscopic data of all chalcones such as absorption maximum λ_{max}(nm) of carbonyl groups, infrared carbonyl stretches of *ν*CO*s-cis* and *s-trans*, the deformation modes of vinyl part CH *out of plane*, *in-plane*, CH=CH and >C=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-(4-isobutylphenyl)-3-phenyl-2-propenone compounds were assigned and presented in **Table-2**. These absorption maxima (λ_{max} nm) of these 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds were correlated with Hammett substituent constants and *F* and *R* parameters using single and multi-linear regression analysis[1, 4, 28-34,37-42] Hammett correlation involving the group frequencies and absorption maxima, the form of the Hammett equation employed is

$$\lambda = \rho\sigma + \lambda_O \qquad \text{… (1)}$$

Where λ_O is the frequency for the parent member of the series.

Table-2. The, UV (λ_{max}) and Infrared absorptions (υ cm^{-1}) spectral data of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds

S.No	Substituents	UV	CO *s-cis*	CO *s- trans*	CH_{ip}	CH_{op}	$CH{=}CH_{op}$	$C{=}C_{op}$
1	H	286.2	1660.70	1598.90	1222.87	829.39	1023.27	514.99
2	3-Br	306.0	1662.64	1595.13	1211.30	788.89	995.27	559.36
3	4-Br	310.3	1658.78	1589.34	1201.65	748.39	1049.28	572.86
4	3-Cl	316.2	1660.71	1600.92	1215.15	788.89	985.62	561.29
5	4-Cl	329.0	1664.57	1593.20	1209.37	790.81	995.21	557.43
6	4-F	323.1	1660.71	1597.06	1222.87	829.30	1020.34	516.92
7	2-OCH_3	306.0	1660.71	1598.99	1220.94	825.53	1020.34	513.07
8	4-CH_3	296.5	1658.78	1589.34	1203.58	750.31	1051.21	576.09
9	3-NO_2	316.5	1658.79	1593.20	1207.44	754.17	1058.92	578.64

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3.2.1 Correlation analysis of UV spectral data of substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds.

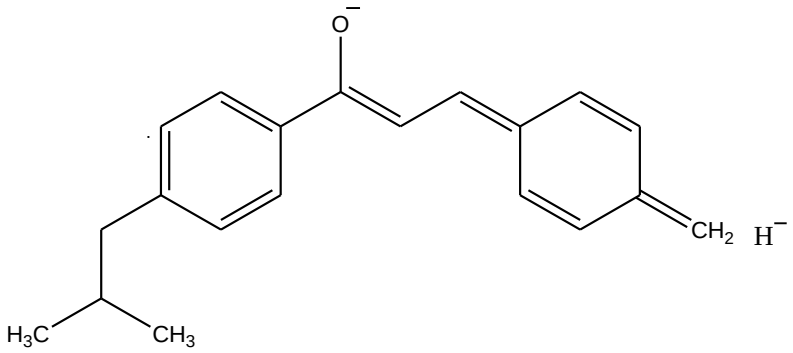
The assigned UV absorption maximum λ_{max} (nm) values of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds are presented in **Table-2**.

These UV absorption maximum values have been correlated with Hammett substituent constants and *F* and *R* parameters using single and multi-linear regression analyses according to approach of John Shorter[38].The results of statistical analysis are presented in **Table-3**.

From **Table-3**, it is evident that the UV absorption maximum λ_{max}(nm) values of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds except that with 4-Cl have shown satisfactory correlations with Hammett substituent constant σ_I (r = 0.901) and *F* (r = 0.900) parameter.

When the substituent that has been given exception when included in regression it reduces the correlations considerably.

The UV absorption maximum λ_{max}(nm) values of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlations (r < 0.900)with remaining Hammett substituent constants σ, σ^+& σ_R and *R* parameter. This is due to the incapability of polar and resonance effects of the substituents for predicting the reactivity on the UV absorption maximum λ_{max} (nm) values through resonance as per the conjugative structure **(1).**



(1)

All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect with respect to UV absorption maximum λ_{max} (nm) values of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds.

Table- 3. The results of statistical analysis of UV λ_{max}(nm) values of substituted *(E)*-1-(4-isobutyl phenyl)-3-phenyl-2-propenone compounds with Hammett substituent constants and *F* and *R* parameters

Absorption maximum	Constants	r	I	ρ	s	n	Correlated derivatives
λ_{max}(nm)	σ	0.840	307.17	16.239	12.95	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.831	308.35	10.703	13.45	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.901	293.03	45.513	8.16	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.823	307.13	14.093	13.75	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.900	293.41	42.944	8.23	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.829	306.35	15.163	13.65	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

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Most of the single regression analyses have shown poor correlations with Hammett substituent constants σ, σ^+& σ_R and *R* parameter, 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 compounds with inductive, resonance and Swain-Lupton's[39] *F* and *R* parameters produce satisfactory correlations as shown in equations **(2)** and **(3).**

$$UV(\lambda_{max}) = 290.982\ (\pm 5.732) + 45.007(\pm 12.267)\sigma_I - 11.945(\pm 12.970)\ \sigma_R \quad \ldots\textbf{(2)}$$

$$(R = 0.984,\ n = 10,\ P > 95\%)$$

$$UV(\lambda_{max}) = 292.723\ (\pm 5.902) + 41.928(\pm 12.731)F - 4.764(\pm 13.732)\ R \quad \ldots\textbf{(3)}$$

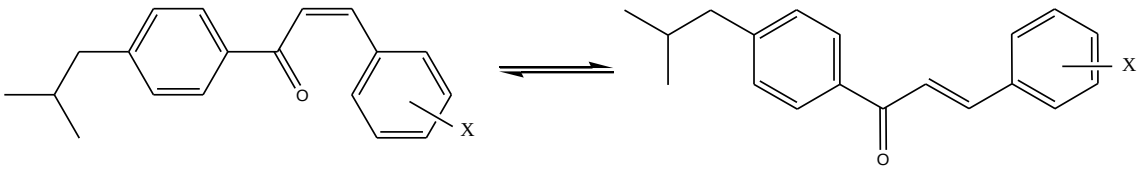
$(R = 0.981,\ n = 10,\ P > 95\%)$

3.3 IR Spectral Study

The assigned νCO(cm^{-1}) stretches of the s-*cis* and *s-trans* conformers and νCH_{ip}, CH_{op}, $CH{=}CH_{op}$ and $C{=}C_{op}$(cm^{-1}) modes of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds are presented in **Table-2** and the corresponding s-*cis* and *s-trans* conformers are shown in **(2).** The stretching frequencies for carbonyl absorption are assigned based on the assignments made by Hays and Timmons[40] for *s-cis* and *s-trans* conformers at 1690 and 1670 cm^{-1}, respectively. These data have been correlated with Hammett substituent constants and Swain-Lupton's constants[39] and are presented in **Table-4**. In this correlation the structure parameter Hammett equation employed is as shown in the following equation:

$$\upsilon = \rho\sigma + \upsilon_0 \qquad \textbf{... (4)}$$

where υ 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.



s-cis ***s-trans***

(2)

These IR frequency values have been correlated with Hammett substituent constants and *F* and *R* parameters according to the approach of Jaffe[41]. The results of the statistical analysis are presented in **Table-4.**

Table-4.The results of statistical analysis of infrared (cm^{-1}) values of $\nu CO_{s\text{-}cis}$, $\nu CO_{s\text{-}trans}$, νCH_{ip}, νCH_{op}, $\nu CH{=}CH_{op}$ and $\nu C{=}C_{op}$ of substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds with Hammett constants and *F* and *R* parameters

Frequency	Constants	r	I	ρ	s	n	Correlated derivatives
$\nu CO_{s\text{-}cis}$(cm^{-1})	σ	0.798	1590.54	-5.344	20.457	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.825	1591.36	-12.63	19.868	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.813	1593.56	-10.537	20.369	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.813	1587.58	-11.179	20.368	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.808	1592.04	-6.188	20.477	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.806	1588.51	-5.207	20.504	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
$\nu CO_{s\text{-}trans}$(cm^{-1})	σ	0.812	1506.17	-10.134	27.437	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.807	1505.27	-4.921	27.596	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.882	1513.59	-24.573	26.955	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.820	1508.90	23.172	27.103	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.812	1509.49	-12.973	27.451	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.815	1508.54	17.699	27.318	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
νCH_{ip}(cm^{-1})	σ	0.836	1214.24	-9.052	8.059	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.840	1213.92	-8.480	7.931	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

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	σ_I	0.817	1214.14	-3.676	8.623	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.850	1209.39	-18.09	7.500	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.800	1212.72	0.2011	8.673	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.844	1209.33	-15.33	7.788	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
Frequency	**Constants**	**r**	**I**	**ρ**	**s**	**n**	**Correlated derivatives**
$\nu CH_{op}(cm^{-1})$	σ	0.845	796.89	-46.08	31.81	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.848	795.11	-42.11	31.21	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.813	796.37	-18.63	35.44	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.858	773.22	-86.75	29.02	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.802	791.03	-3.969	35.74	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.852	772.62	-74.90	30.50	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
$\nu CH{=}CH_{op}(cm^{-1})$	σ	0.801	1022.38	-1.402	28.589	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.801	1022.01	1.108	28.589	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.815	1028.57	-17.42	28.247	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.831	1029.41	38.62	27.04	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.807	1025.37	-8.430	28.503	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.821	1029.27	31.51	27.495	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
$\nu C{=}C_{op}(cm^{-1})$	σ	0.860	542.13	49.56	23.36	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.861	544.43	42.45	23.34	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.823	540.21	26.79	28.41	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.862	564.43	76.46	22.69	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.810	545.69	11.49	29.05	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.857	565.17	66.94	24	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

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

3.3.1 Correlation analysis of IR spectral data substituted 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

From **Table-4**, it is evident that the infrared stretching frequency **$\nu CO_{s\text{-}cis}(cm^{-1})$, $\nu CO_{s\text{-}trans}(cm^{-1})$, $\nu CH_{ip}(cm^{-1})$, νCH_{op} (cm^{-1}), $\nu CH{=}CH_{op}(cm^{-1})$** and **$\nu C{=}C_{op}(cm^{-1})$** values of all the *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds have shown poor correlation (r < 0.900) with all the Hammett substituent constant σ, σ^+, σ_I and σ_R and *F* and *R* parameters. This is attributed to the weakpolar, inductive, field and resonance effects of the substituents for predicting the reactivity on the infrared frequencies through resonance as per the conjugative structure **(1).**

Most of the correlations of the infrared stretching frequency **$\nu CO_{s\text{-}cis}(cm^{-1})$, $\nu CO_{s\text{-}trans}(cm^{-1})$, $\nu CH_{ip}(cm^{-1})$, νCH_{op} (cm^{-1})** and **$\nu CH{=}CH_{op}(cm^{-1})$** have shown negative ρ values with all the Hammett substituent constants and *F* & *R* parameters. This indicates the operation of reverse substituent effect with respect to the infrared frequency values of the entire *(E)*-

1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

All the correlations of the infrared stretching frequency **$\nu C{=}C_{op}(cm^{-1})$** have shown positive ρ values with most of the Hammett substituent constants σ, σ_I and σ_R and *F* and *R* parameters. This indicates the operation of normal substituent effect with respect to infrared frequency values of all the *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

In this case all the single regression analyses have shown poor correlations with Hammett substituent constants and *F* and *R* parameters. Hence, it is decided to go for multi regression analysis. The multi regression analysis of the infrared frequency **$\nu CO_{s\text{-}cis}(cm^{-1})$, $\nu CO_{s\text{-}trans}(cm^{-1})$, $\nu CH_{ip}(cm^{-1})$, νCH_{op} (cm^{-1}), $\nu CH{=}CH_{op}(cm^{-1})$** and **$\nu C{=}C_{op}(cm^{-1})$** values of all the compounds with inductive, resonance and Swain-Lupton's[39]parameters have shown satisfactory correlations as shown in equations **(5)** - (**6)**.

$$\nu CO_{s\text{-}cis}(cm^{-1}) = 1589.77(\pm15.258) - 14.667(\pm25.868)\sigma_I + 5.067(\pm42.081)\ \sigma_R \quad \ldots\textbf{(5)}$$
$$(R = 0.929,\ n = 9,\ P > 90\%)$$

$$\nu CO_{s\text{-}cis}(cm^{-1}) = 1591.016(\pm14.775) - 7.706(\pm31.872)F - 7.118(\pm34.379)R \quad \ldots\textbf{(6)}$$
$$(R = 0.918,\ n = 9,\ P > 90\%)$$

$$\nu CO_{s\text{-}trans}(cm^{-1}) = 1517.386(\pm19.831) - 23.632(\pm42.440)\sigma_I + 22.044(\pm44.871)\ \sigma_R \quad \ldots\textbf{(7)}$$
$$(R = 0.927,\ n = 9, P > 90\%)$$

$$\nu CO_{s\text{-}trans}(cm^{-1}) = 1511.706(\pm19.831) - 9.713(\pm42.485)F + 15.290(\pm45.822)\ R \quad \ldots\textbf{(8)}$$
$$(R = 0.902,\ n = 9,\ P > 90\%)$$

$$\nu CH_{ip}(cm^{-1}) = 1210.997(\pm5.563) - 4.458(\pm11.906)\sigma_I - 18.310(\pm12.588)\ \sigma_R \quad \ldots\textbf{(9)}$$
$$(R = 0.982,\ n = 9,\ P > 95\%)$$

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$\nu CH_{ip}(cm^{-1}) = 1210.391(\pm5.606) - 3.239(\pm12.092)F + 16.139(\pm13.042)R$ ... **(10)**
(R = 0.957, n = 9, P > 95%)

$\nu CH_{op}(cm^{-1}) = 781.261(\pm21.357) - 22.385(\pm45.705)\sigma_I - 87.824(\pm48.324)\ \sigma_R$ …**(11)**
(R = 0.972, n = 9, P > 95%)

$\nu CH_{op}(cm^{-1}) = 779.470(\pm21.728) - 21.052(\pm46.870)F - 80.120(\pm50.551)R$ …**(12)**
(R = 0.978, n = 9, P > 95%)

$\nu CH{=}CH_{op}(cm^{-1}) = 1035.088(\pm20.064) - 15.812(\pm42.938)\sigma_I + 37.867(\pm45.398)\ \sigma_R$…**(13)**
(R = 0.969, n = 10, P > 95%)

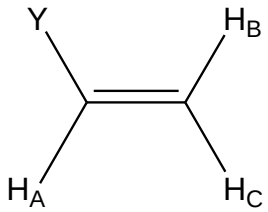
$\nu CH{=}CH_{op}(cm^{-1}) = 1029.860(\pm19.907) - 1.814(\pm42.940)F + 31.064(\pm46.314)R$ …**(14)**
(R = 0.941, n = 10, P > 90%)

$\nu C{=}C_{op}(cm^{-1}) = 553.620(\pm16.032) + 30.116(\pm34.310)\ \sigma_I + 77.906(\pm36.276)\ \sigma_R$ …**(15)**
(R = 0.994, n = 10, P > 95%)

$\nu C{=}C_{op}(cm^{-1}) = 556.327(\pm16.599) + 27.203(\pm37.805)F + 73.695(\pm38.618)R$ …**(16)**
(R = 0.945, n = 10, P > 90%)

3.4 ^{1}H NMR Spectral Studies

From the ^{1}H NMR spectra of synthesised 1-(4-isobutylphenyl)-3-phenyl-2-propenone 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 **(3).**The β proton doublet in most cases is well separated from aromatic protons.



(3)

Solcaniova and Toma[42] have investigated the effect of substituent on the ^{1}H 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[42]observed opposite sign of the slopes for H_α and H_β in their correlations of chemical shift with substituent constants . 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-(4-isobutylphenyl)-3-phenyl-2-propenone 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).**

$$\delta = \rho\sigma + \delta_o \quad \text{… (17)}$$

where $\boldsymbol{\delta_o}$ is the ^{1}H NMR chemical shift of the corresponding parent compound.

3.4.1 Correlation analysis of ^{1}H NMR spectral data of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

The assigned ^{1}H NMR chemical shift δH_α(ppm) and δH_β(ppm) values of all the substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds are presented in **Table-5**. These observed ^{1}H NMR chemical shift δH_α(ppm) and δH_β(ppm) values have been correlated with Hammett substituent constants and *F* and *R* parameters. The results of statistical analysis are shown in **Table-6**.

Table-5. The ^{1}H-NMR, 13C-NMR (ppm) and UV (λ_{max}nm) spectral data of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

S. No	Substituents	H_α	H_β	C_α	C_β	CO
1	H	7.588	7.840	122.19	144.37	190.12
2	3-Br	7.747	7.813	127.23	133.12	189.60

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3	4-Br	7.760	7.970	122.68	142.89	189.78
4	3-Cl	7.562	7.750	123.33	136.89	189.56
5	4-Cl	7.542	7.785	122.53	135.74	189.76
6	4-F	7.500	7.807	121.85	143.03	189.88
7	2-OCH_3	7.508	7.807	121.85	135.83	190.16
8	4-CH_3	7.548	7.836	121.16	144.46	190.19
9	3-NO_2	7.654	7.842	122.29	141.16	189.20

From **Table-6**, it is evident that the ^{1}H NMR chemical shift **δH_α (ppm)** and **δH_β (ppm)** values of all the *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds have shown poor correlation (r< 0.900) with Hammett substituent constants and *F* and *R* parameters.

This is attributed to the weak inductive and field effects of the substituents for predicting the reactivity on the ^{1}H 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 ^{1}H NMR chemical shift **δH_α(ppm)** and **δH_β(ppm)** values of all the *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds.

In this case all the single regression analyses have shown poor correlations with Hammett substituent constant and *F* and *R* parameter. So, it is decided to go for multi regression analysis. The multi regression analysis of ^{1}H NMR chemical shift **δH_α(ppm)** and **δH_β(ppm)** values of all the *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds with inductive, resonance and Swain-Lupton's[39] parameters produce satisfactory correlations as shown in equations **(18) - (21).**

$$\delta H_\alpha(\text{ppm}) = 7.587(\pm.061) + 0.141(\pm0.132)\sigma_I + 0.228\pm(0.140)\sigma_R \quad \ldots\textbf{(18)}$$

$$(R = 0.917, n = 10, P > 95\%)$$

$$\delta H_\alpha(\text{ppm}) = 7.600(\pm0.064) + 0.117(\pm0.138)F + 0.216(\pm0.149)R \quad \ldots\textbf{(19)}$$

$(R = 0.910, n = 10, P > 95\%)$

$$\delta H_\beta(\text{ppm}) = 7.838(\pm0.048) - 0.009(\pm0.103)\sigma_I + 0.079(\pm0.108)\sigma_R \quad \ldots\textbf{(20)}$$

$$(R = 0.989, n = 10, P > 95\%)$$

$$\delta H_\beta(\text{ppm}) = 7.835(\pm0.047) + 0.0034(\pm0.101)F - 0.059(\pm0.109)R \quad \ldots\textbf{(21)}$$

$$(R = 0.894, n = 10, P > 95\%)$$

Table-6. The results of statistical analysis of ^{1}H NMR chemical shift δH_α(ppm) and δH_β(ppm) values of Substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds with Hammett substituent constants σ, σ^+, σ_I & σ_R and *F* and *R* parameters.

Chemical shifts	Constants	r	I	ρ	s	n	Correlated derivatives
δH_α(ppm)	σ	0.858	7.568	0.173	0.084	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.871	7.572	0.180	0.073	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.832	7.548	0.131	0.099	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.851	7.638	0.221	0.090	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.818	7.569	0.071	0.102	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.844	7.638	0.187	0.093	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
δH_β(ppm)	σ	0.808	7.82	0.015	0.066	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.824	7.818	0.039	0.064	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.801	7.824	-0.004	0.066	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.824	7.838	0.079	0.064	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.803	7.826	-0.009	0.066	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.821	7.836	0.059	0.065	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

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

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3.5 ^{13}C NMR Spectral Study

Dhami and Stothers[43] have made extensive study of ^{13}C NMR spectra of a large number of different acetophenones and styrenes. They found a linear correlation of the chemical shift of the CO carbons with Hammett σ constants in styrene.

The assignment of chemical shift for the ethylenic carbons is based on the following consideration. In mono substituted styrenes, the α-carbon (nearer to phenyl ring) falls in a quite well-defined region, 133-138ppm. Compounds the carbon atom is considered as C_β whose chemical shift fall in the region 137-145ppm.

The low field absorption is caused by the electron withdrawing aryl group attached to neighboring carbon. The other carbon of ethylenic bond C_α lies relatively at higher field (118-126 ppm) than the corresponding carbon in styrenes.

Based on this hypothesis, it is attempted in the present investigation, to determine to what extent ^{13}C chemical shift reflect the electronic influence of substituents, and also to interpret the transmission of substituent effects on CO, C_α and C_β carbons in substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds. The assignment of ^{13}C NMR, chemical shift (ppm) values of carbonyl carbon, C_α and C_β of all the synthesised *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-one compounds are presented in **Table-5.** The results of statistical analysis are given in **Table-7**.

3.5.1 Correlation analysis of ^{13}C- NMR spectral data of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

From **Table-7**, it is evident that the **δCO** chemical shift (ppm) of all the *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds with all the substituents have shown satisfactory correlation with Hammett substituent constants σ(r = 0.958), σ^+(r = 0.925) and σ_I(r = 0.918). The remaining Hammett constant σ_R and *F* and *R* parameters have shown poor correlations (r<0.900) with δCO chemical shift (ppm) values.

The **δC_α** and **δC_β** chemical shifts (ppm) values of all the *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds have shown poor correlations (r < 0.900) with all the Hammett substituent constants namely σ,σ^+, σ_I and σ_R and *F* and *R* parameters.

This is attributed to the weak polar, field and resonance effect of the substituents for predicting the reactivity on the ^{13}CNMR chemical shift through resonance as per the conjugative structure **(1).** The correlations values of **δCO** and **δC_β** has shown negative ρ values indicates operation of reverse substituent effect and **δC_α** has shown positive ρ values indicates operation of normal substituent effect with Hammett substituent constants and *F* and *R* parameters.

Table-24. The results of statistical analysis of ^{13}C NMR chemical shift δCO(ppm), δC_α(ppm) and δC_β(ppm) values of substituted *(E)*-1-(4-isobutylphenyl)-3-phenylprop-2-en-1-onecompounds (series-D)with Hammett substituent constants σ, σ^+, σ_I & σ_R and *F* and *R* parameters.

Chemical shifts	Constants	r	I	ρ	s	n	Correlated derivatives
δCO (ppm)	σ	0.958	189.95	-0.943	0.0987	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.925	189.90	-0.776	0.134	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.918	190.21	-1.113	0.202	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.849	189.67	-0.717	0.302	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.869	190.15	-0.907	0.249	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.846	189.65	-0.656	0.307	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
δC_α (ppm)	σ	0.844	122.41	2.364	1.699	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.847	122.50	2.16	1.669	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.833	121.88	2.458	1.788	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.812	122.97	1.011	1.878	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

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	F	0.821	122.21	1.498	1.851	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.809	122.95	0.721	1.885	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
δC_β (ppm)	σ	0.815	140.05	-2.067	4.566	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ^+	0.813	139.91	-1.472	4.584	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_I	0.841	141.46	-7.458	4.217	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	σ_R	0.827	140.71	5.284	4.446	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	F	0.824	141.30	-4.164	4.487	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2
	R	0.819	140.54	3.633	4.535	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3, 4-CH_3, 3-NO_2

r = correlation co-efficient; ρ = slope; I = Intercept; s = standard deviation; n = number of substituents
Some of the single parameter correlations are shown in **Fig: (2) - (4).**

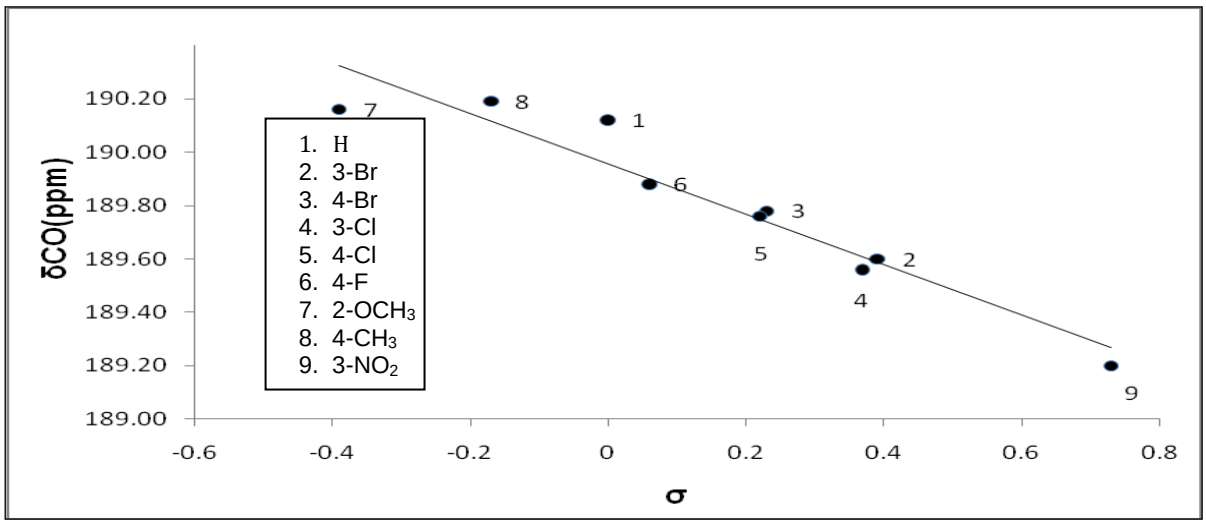

Fig-2. Plot of δCO chemical shift (ppm)values of substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds Vs σ

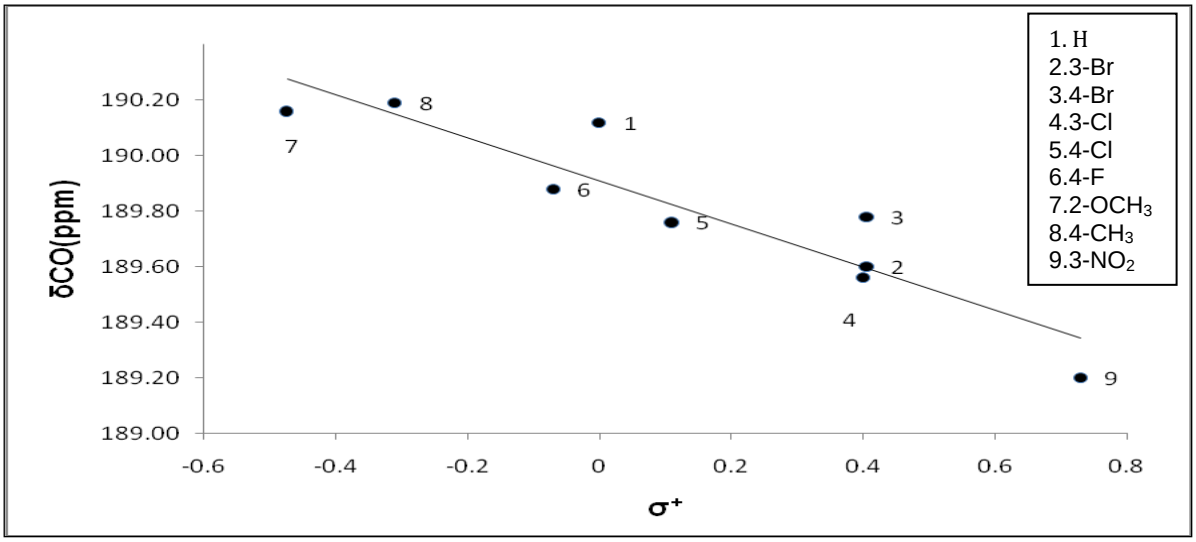

Fig-3. Plot of δCO chemical shift (ppm) values of substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds Vs σ^+

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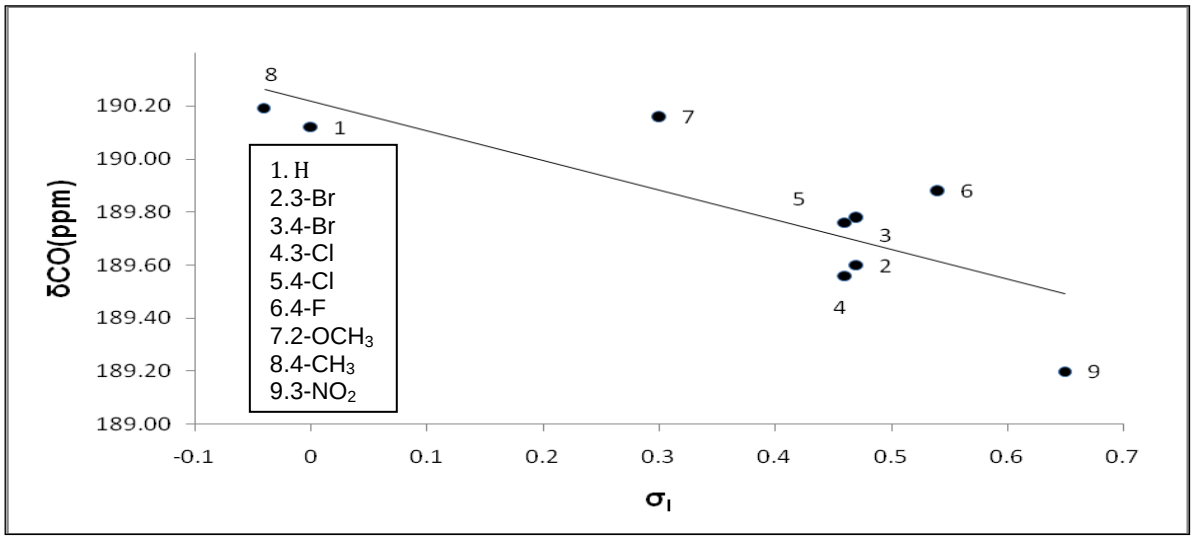

Fig-4. Plot of δCO chemical shift (ppm) values of substituted *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds Vs σ_I

In this case some of the single regression analyses have shown poor correlations with a few Hammett substituent constant σ_R and *F* and *R* parameters. So, it is decided to go for multi regression analysis. The multi regression analysis of the **δCO**, **δC_α** and **δC_β** chemical shift (ppm) values of all the *(E)*-1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds with inductive, resonance and Swain-Lupton's[39]parameters produce satisfactory correlations as shown in equations**(22) - (27).**

$\delta CO(ppm) = 190.082(\pm0.062) - 1.146(\pm1.130)\sigma_I - .0.772(\pm0.137)\sigma_R$ …**(22)**

(R = 0.933, n = 10, P > 90%)

$\delta CO\ (ppm) = 190.017(\pm0.076) - 1.105(\pm.164)F + 0.930(\pm0.177)R$ …**(23)**

(R = 0.914, n = 10, P > 90%)

$\delta C_\alpha\ (ppm) = 122.08\ (\pm1.326) + 2.506(\pm2.837)\sigma_I + 1.131(\pm3.004)\sigma_R$ …**(24)**

(R = 0.936, n = 10, P > 90%)

$\delta C_\alpha\ (ppm) = 122.385\ (\pm1.325) + 1.744(\pm2.858)F + 1.153(\pm8.082)R$ …**(25)**

(R = 0.925, n = 10, P > 90%)

$\delta C_\beta\ (ppm) = 143.314\ (\pm3.036) - 7.248(\pm6.497)\sigma_I + 4.938(\pm6.870)\sigma_R$ …**(26)**

(R = 0.928, n = 10, P > 90%)

$\delta C_\beta\ (ppm) = 141.704\ (\pm3.213) - 3.579(\pm6.931)F + 2.746(\pm7.476)R$ …**(27)**

(R = 0.953, n = 10, P > 95%)

4. ANTIMICROBIAL ACTIVITY

4.1 Antibacterial Activity

The newly synthesized chalcones (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 Kirby Bauer disc diffusion method[31] **(Plate 1- 6)**. 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 5 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 37^0C for 24 Hour.

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A reference standard drug of gram positive and gram negative bacteria was made by dissolving 5.0 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-8.**

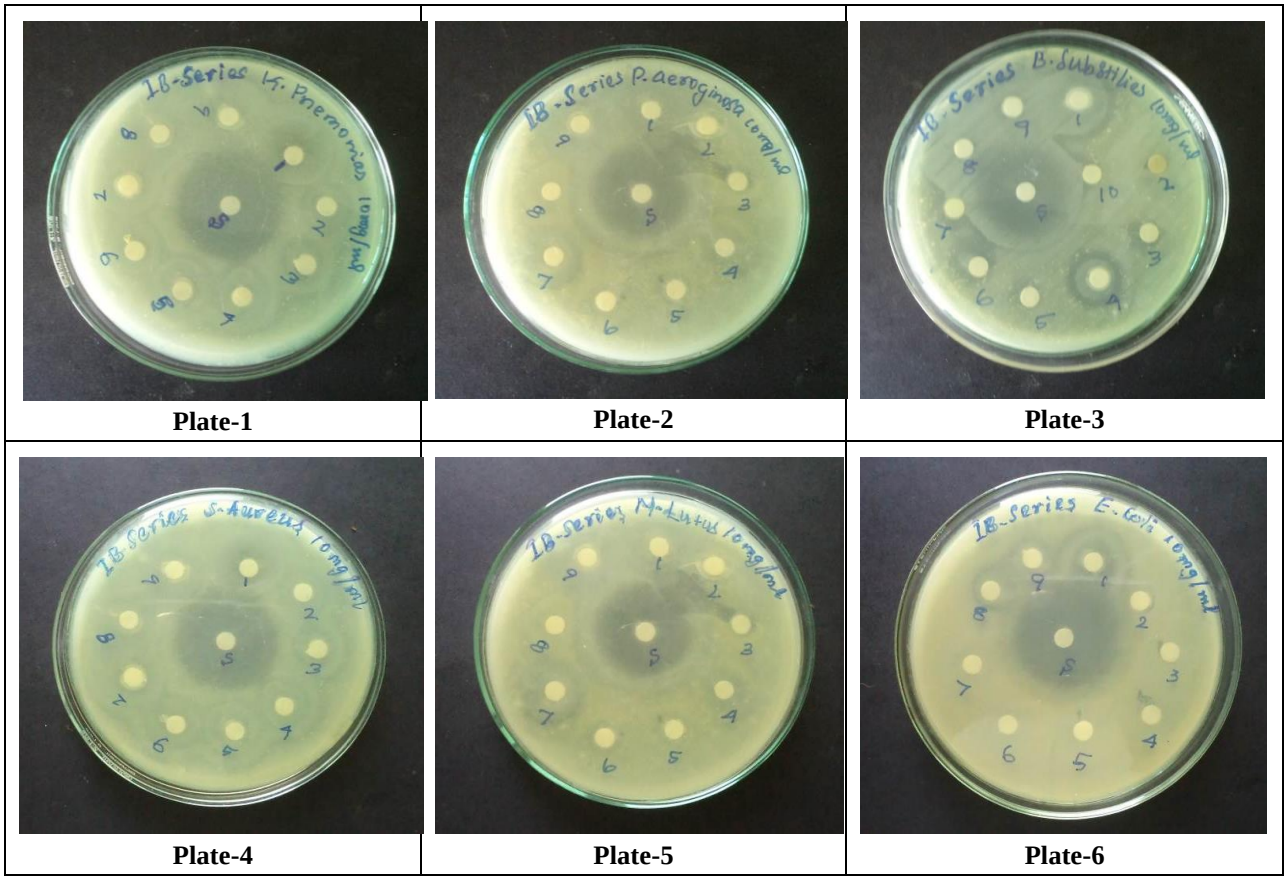

Fig-5. The antibacterial images of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

4.1.1 Antibacterial activity against *Bacillus subtilis*

Analysis of the zone of inhibition (mm) values reveals that only one compound with 3-NO_2 substituent in this series has shown excellent antibacterial activity. Three compounds with 4-Br,3-Cl and 4-F substituent has shown good antibacterial activity. Four compounds with H (parent), 3-Br, 2-OCH_3 and 4-CH_3 substituents have shown moderate antibacterial activity. The remaining only one compound with 4-Cl substituent has shown poor antibacterial activity.

4.1.2 Antibacterial activity against *Micrococcus luteus*

Only one compounds with 3-Cl substituent has shown good antibacterial activity. Six compounds with H (parent), 3-Br, 4-Cl, 4-F, 4-CH_3 and 3-NO_2 substituents has shown moderate antibacterial activity. The remaining two compounds with 4-Br and 2-OCH_3 substituents has shown poor antibacterial activity.

4.1.3 Antibacterial activity against Staphylococcus aureus

Only one compound with 2-OCH_3 substituent has shown good antibacterial activity. The 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F and 4-CH_3 substituted compounds has shown moderate antibacterial activity. The remaining two compounds with H (parent) and 3-NO_2 substituents has shown poor antibacterial activity.

4.1.4 Antibacterial activity against *Escherichia coli*

Three compounds with H (parent), 4-CH_3 and 3-NO_2substituents has shown good antibacterial activity. The 3-Br, 4-Br, 3-Cl and 4-Cl, substituted compounds in this series has shown moderate antibacterial activity. The remaining two compounds with and 4-F and 2-OCH_3 substituents has shown poor antibacterial activity.

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4.1.5 Antibacterial activity against *Pseudomonas aeruginosa*

Two compounds with H (parent) and 3-NO_2 substituent in this series has shown good antibacterial activity. The remaining seven compounds with 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 2-OCH_3 and 4-CH_3 substituents has shown moderate antibacterial activity.

4.1.6 Antibacterial activity against *Klebsiella pneumoniae*

Two compounds with 4-Br and 2-OCH_3 substituent in this series has shown good antibacterial activity. The remaining seven compounds with H (parent), 3-Br, 3-Cl, 4-Cl, 4-F, 4-CH_3 and 3-NO_2 substituents has shown moderate antibacterial activity.

Table-8. Antibacterial activity of 1-(4-isobutylphenyl)-3-phenyl propenone compounds.

S. No	Substituent	Zone of Inhibition (mm)					
		Gram positive Bacteria			Gram negative Bacteria		
		B.subtilis	*M.luteus*	*S.aureus*	*E.coli*	*P.aeruginosa*	*k.pneumonias*
1	H	6	6	0	8	8	7
2	3-Br	6	6	6	6	6	7
3	4-Br	8	0	6	6	6	8
4	3-Cl	8	8	6	7	6	7
5	4-Cl	0	6	6	7	7	7
6	4-F	9	6	6	0	6	6
7	2-OCH_3	6	0	8	0	7	8
8	4-CH_3	6	6	6	8	7	6
9	3-NO_2	11	6	0	9	8	7
Standard	Ampicillin	13	8	9	12	12	15
control	DMSO	0	0	0	0	0	0

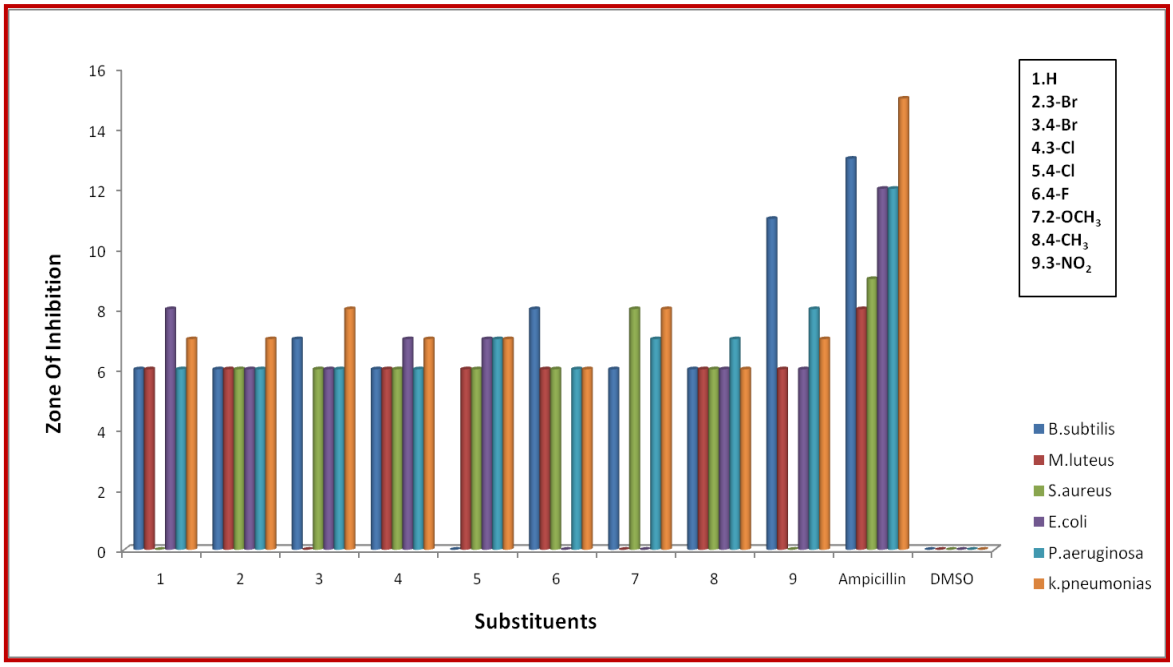

Fig-6. The antibacterial-clustered column chart of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

4.2 Antifungal Activity

All the those compounds screened for antibacterial activity were also tested for antifungal activity using potato–dextrose-agar (PDA) medium same cup and plate method against *Aspergillus niger*, *Tricoderma viride* and *Mucor species* **(Plate 7-**

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9). Preparation of nutrient broths, subculture, base layer medium and PDA-medium was done as per the standard procedure. A reference standard drug fluconazole 5mg 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 presented in **Table-9.**

Table-9. Antifungal activity of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

S.No	Substitution	Mean zone of inhibition (mm)		
		A. Niger	*T. Viride*	*M. Species*
1	H	6	0	7
2	3-Br	9	6	7
3	4-Br	0	8	8
4	3-Cl	0	0	0
5	4-Cl	0	6	0
6	4-F	6	0	6
7	2-OCH_3	6	9	6
8	4-CH_3	0	0	0
9	3-NO_2	8	6	0
Control	DMF	0	0	0
Standard	Fluconazole	12	9	9

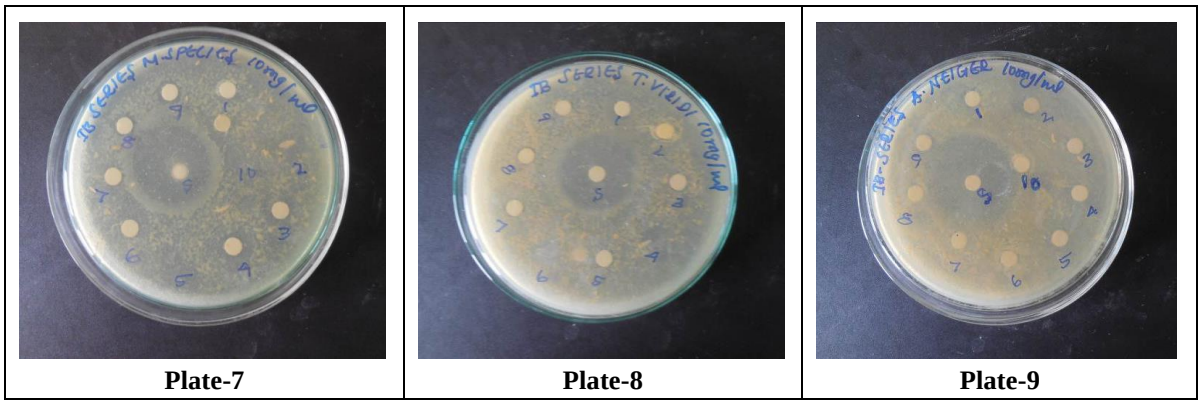

Plate-7 **Plate-8** **Plate-9**

Fig-7.The anti fungal images of substituted 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

4.2.1 Antifungal activity against *Aspergillus niger*

Analysis of the Zone of inhibition (mm) values reveals that the two compounds with 3-Br and 3-NO_2 substituents in this series has shown good antifungal activity. Three compounds with H (parent), 4-F and 2-OCH_3substituents has shown moderate antifungal activity. The remaining four compounds with 4-Br, 3-Cl, 4-Cl and 4-CH_3 substituents has shown poor antifungal activity.

4.2.2 Antifungal activity against *Trichoderma viride*

Two compounds with 4-Br and 2-OCH_3 substituents in this series has shown good antifungal activity. Three compounds with 3-Br, 4-Cl, and 3-NO_2substituents have shown moderate antifungal activity. The remaining four compounds with H (parent),3-Cl, 4-F and 4-CH_3 substituents have shown poor antifungal activity.

4.2.3 Antifungal activity against *Mucor Species*

Only one compound with 4-Br substituent in this series has shown good antifungal activity. Four compounds with H (parent),3-Br, 4-F and2-OCH_3substituents has shown moderate antifungal activity. The remaining four compounds with 3-Cl, 4-Cl, 4-CH_3, and 3-NO_2substituents have shown poor antifungal activity.

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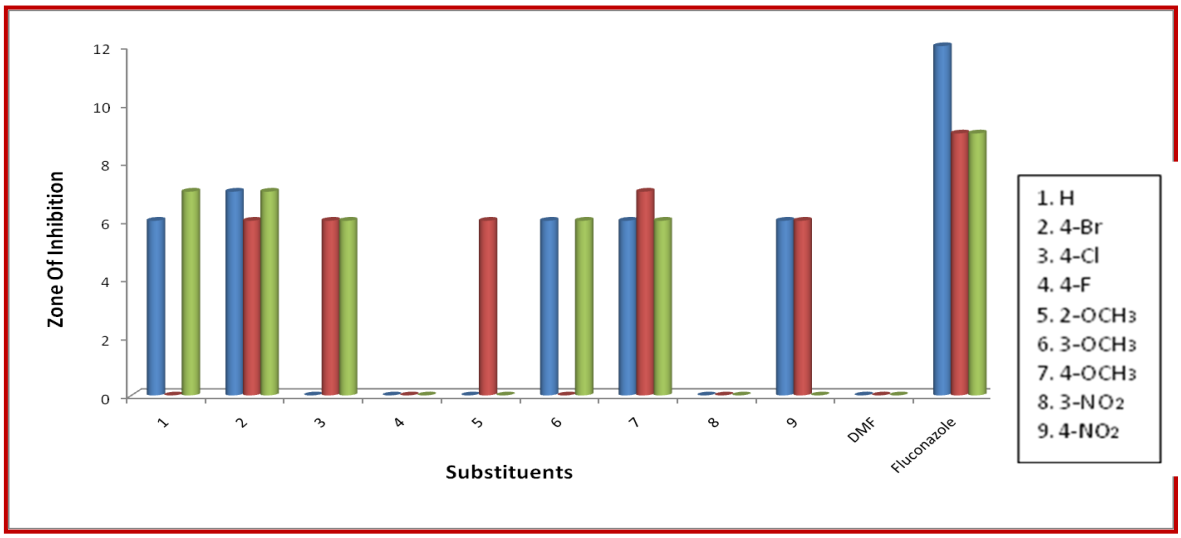

Fig-8.The anti fungal-clustered column chart of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds.

5. CONCLUSION

Some of 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds have been synthesized by condensation of 4-isobutyl acetophenone with substituted benzaldehyde using thionyl chloride-ethanol catalyst by crossed-Aldol condensation method. This reaction protocol offers a simple, easier work-up procedure and good yields. The synthasised 1-(4-isobutylphenyl)-3-phenyl-2-propenone compounds have been characterized by their physical constants, spectral data. The UV, IR, NMR spectral data of these compounds has been correlated with Hammett substituent constants, *F* and *R* parameters. From the results of statistical analyses the effects of substituent on the spectral data have been studied. The antimicrobial activities of all synthesized compounds have been studied using Kirby-Bauer disc diffusion method. The screening results revealed that most of the compounds of this series shown good antibacterial activity. Only few H (parent), 3-Br and 2-OCH_3 substituted compounds shown moderate anti fungal activity and the remaining compounds shown poor antifungal activity.

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