

Spectral Correlations of Antimicrobial Active (*E*)-3,4-Dimethoxyphenyl Enones

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Abstract

*In this work, authors synthesized (*E*)-3,4-dimethoxyphenyl enones by cross-aldol condensation of 3,4-dimethoxyacetophenone with various substituted benzaldehydes in the presence base (sodium hydroxide) using Ultrasound irradiation technique. The synthesized (*E*)-3,4-dimethoxyphenyl enones were characterized by their physical constants, UV, FT-IR, ¹H-NMR & ¹³C-NMR spectral data. All the observed spectral data of substituted (*E*)-3,4-dimethoxyphenyl enones have been correlated with Hammett substituent constants (σ , σ^+ , σ_I & σ_R) and *F* and *R* parameters using single and multi-linear regression analyses. Antimicrobial activities of these enones have been studied and compared with the standard drug ampicillin. Some compounds of the series exhibit anti-microbial activities.*

Keywords: (*E*)-3,4-dimethoxyphenyl enones, IR and NMR spectra, Hammett equation, Substituent effect, Antimicrobial activities.

1. Introduction

Chalcones is a universal term given to compounds bearing the 1, 3-diphenylprop-2-en-1-one framework and belong to the flavonoid family [1-3]. Chemically they are open-chain flavonoids in which the two aromatic rings are joined by a three carbon α , β -unsaturated carbonyl system. 1, 3-diphenylprop-2-en-1-ones are abundantly present in nature starting from ferns to higher plants [4] and a number of them are polyhydroxylated in the aryl rings. In plants, 1,3-diphenylprop-2-en-1-ones are converted to the corresponding (2*S*)-flavanones in a stereospecific reaction catalyzed by the enzyme *chalcone isomerase*. This close structural and biogenetic relationship between chalcones and flavanones explains why they often co-occur as natural products. In the countries such as china, Korea and japan, tetrahydroxy chalcone (a butein) has been traditionally used for treatment of pain thrombotic disease, stomach, gastric, cancer and parasitic as well as food additives [5]. All 1,3-diphenylprop-2-en-1-ones are well known intermediates for synthesizing various heterocyclic compound .the compounds with the backbone of biological activities such as anti-inflammatory [6-8], antimitotic [9], anti-leishmanial [10], anti-invasive [11,12], anti-tuberculoid [13], anti-fungal [14], anti-malarial [15,16], anti-tumor, and anti-oxidant properties [17] as well as their recognized synthetic utility in the preparation of pharmacologically-interesting heterocyclic systems like pyrazolines, which have also been largely studied owing to their pharmacological activities, which includes anti-tumor [18], anti-inflammatory [19], anti-parasite [20], anti-depressive, anticonvulsant [21], antimicrobial [22], anti-nociceptive [23] and nitric oxide synthase inhibitors, associated with diseases such as Alzheimer, Huntington, and inflammatory arthritis [24]. The presence of a reactive and unsaturated carbonyl function in 1, 3-diphenylprop-2-en-1-one is found to be responsible for their antimicrobial activity. Recently, Balaji [25], Sekar [26] and Mala et al.,[27] have synthesized and investigated the catalytic activity and pharmaceutical effects of (*E*)-1-(2,4-dimethylthiazol-5-yl)-3-phenylprop-2-en-1-ones, pyrenyl and triphenyl styryl ketones. Literature survey shows that there is no information available regarding the study of UV, IR and NMR spectral data and spectral correlation of substituted (*E*)-3,4-dimethoxyphenyl enones. In view of this, we have reported the ultrasound irradiated synthesis, quantitative structure activity relationships through Hammett correlations and biological activities of substituted (*E*)-3,4-dimethoxyphenyl enones.

2. Materials and Methods

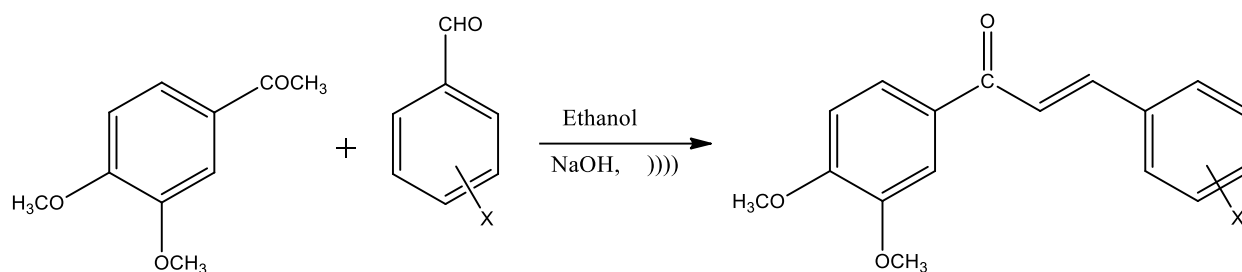
2.1. General

All the used chemicals were purchased from E-Merck, Sigma-Aldrich, and Himedia chemical companies. Melting points of all synthesized substituted (*E*)-3,4-dimethoxyphenyl enones were observed in open glass capillaries on Mettler FP51 melting point apparatus and were uncorrected. The Shimadzu-1650 ultraviolet spectrophotometer was utilized for recording the absorption maxima (λ_{max} , nm), of all substituted (*E*)-3,4-dimethoxyphenyl enones in spectral grade methanol. Infrared spectra (KBr, 4000–400 cm^{-1}) of all substituted (*E*)-3,4-dimethoxyphenyl enones were recorded in Avatar-300 Fourier transform spectrophotometer. The NMR spectra of all substituted (*E*)-3,4-dimethoxyphenyl enones were recorded in Bruker

AV400 NMR spectrometer, operating 400 MHz for ^1H and 100 MHz for ^{13}C spectra in CDCl_3 solvent using TMS as internal standard.

2.2. General procedure for synthesis (*E*)-3,4-dimethoxyphenyl enones

Substituted styryl 3,4-dimethoxy phenyl ketones were prepared by Ultra sonication method. A mixture of 3,4-dimethoxyacetophenone (0.05 mol), various substituted benzaldehydes (0.05 mol), 10 ml of ethanol and 0.5 ml of 1N NaOH were sonicated for 4-9 minutes in a Sonicator at room temperature (CITIZEN Ultra Sonicator, 120W, 40 Hz, 230V Ac) (**Scheme-1**). Performance of the reaction was monitored by thin layer chromatogram. The obtained crude (*E*)-3,4-dimethoxyphenyl enones were filtered at pump, washed with water dried in air-oven and recrystallized from rectified spirit to get glittering yellow color solid. The physical constants are presented in **Table 1**. The UV, IR and NMR spectral value of these substituted (*E*)-3,4-dimethoxyphenyl enones are presented in **Table 2**.



X= H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-OCH₃, 4-CH₃, 4-NO₂

Scheme-1: Synthesis of substituted (*E*)-3,4-dimethoxyphenyl enones.

Table 1. Physical constants of substituted (*E*)-3,4-dimethoxyphenylprop-2-en-1-ones

Entry	X	M. F.	M. W.	Yield (%)	Time (m)	m.p. (°C)[28]
1	H	C ₁₇ H ₁₆ O ₃	268	88	4	74-75
2	3-Br	C ₁₇ H ₁₅ BrO ₃	347	82	5	94-95
3	4-Br	C ₁₇ H ₁₅ BrO ₃	347	83	6	92-93
4	3-Cl	C ₁₇ H ₁₅ ClO ₃	303	83	5	62-63
5	2-F	C ₁₇ H ₁₅ FO ₃	286	80	7	75-76
6	4-F	C ₁₇ H ₁₅ FO ₃	286	80	6	92-93
7	4-OCH ₃	C ₁₈ H ₁₈ O ₄	298	90	4	76-77
8	4-CH ₃	C ₁₈ H ₁₈ O ₃	282	88	7	68-69
9	4-NO ₂	C ₁₇ H ₁₅ NO ₅	313	80	9	122-123

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

Entry	X	UV (λ_{max} , nm)	IR (ν , cm^{-1})					
			CO <i>cis</i>	CO <i>trans</i>	CH _{<i>ip</i>}	CH _{<i>op</i>}	CH=CH _{<i>op</i>}	C=C _{<i>op</i>}
1	H	317.40	1664.23	1605.56	1164.20	759.11	979.83	487.94
2	3-Br	300.20	1653.25	1596.90	1145.62	787.02	1020.34	561.04

3	4-Br	308.50	1655.82	1600.36	1145.15	758.25	1019.67	591.63
4	3-Cl	309.60	1650.31	1577.65	1160.23	777.62	1021.53	563.49
5	2-F	312.20	1651.56	1597.54	1164.84	768.58	1021.96	585.29
6	4-F	310.20	1651.92	1576.43	1161.76	805.23	1017.54	507.52
7	4-CH ₃	335.20	1654.76	1599.29	1149.52	805.09	1020.78	500.37
8	4-OCH ₃	344.60	1650.47	1594.78	1161.34	796.18	1026.46	555.49
9	4-NO ₂	317.60	1655.28	1597.52	1150.26	755.35	1018.39	594.82
Entry	X	¹ H NMR (δ, ppm)		¹³ C NMR (δ, ppm)				
		H _α	H _β	C _α	C _β	CO		
1	H	7.563	7.814	121.69	144.03	188.66		
2	3-Br	7.591	7.773	122.89	142.17	188.16		
3	4-Br	7.734	7.747	122.16	142.57	196.92		
4	3-Cl	7.552	7.732	124.85	142.26	188.18		
5	2-F	7.677	7.899	124.49	149.29	188.64		
6	4-F	7.492	7.772	123.03	142.70	188.40		
7	4-CH ₃	7.521	7.804	122.98	144.13	188.77		
8	4-OCH ₃	7.447	7.791	122.86	143.86	188.66		
9	4-NO ₂	7.510	7.660	123.37	140.74	196.26		

3. Result and Discussion

3.1. Spectral linearity

The spectral linearity of substituted (*E*)-3,4-dimethoxyphenyl enones were studied for evaluating the substituent effects [29, 30] with respect to various spectral data. The assigned spectral data of all substituted (*E*)-3,4-dimethoxyphenyl enones such as absorption maximum λ_{max} (nm), infrared carbonyl stretches of ν_{CO} *s-cis* and ν_{CO} *s-trans*, the deformation modes of 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 Hammett substituent constants (σ , σ^+ , σ_I , σ_R) [29, 30] and *F* and *R* parameters [31].

3.1.1. UV spectral study

The absorption maxima (λ_{max} nm) of synthesized substituted (*E*)-3,4-dimethoxyphenyl enones were assigned and presented in Table 2. These absorption maxima (λ_{max} nm) of these substituted (*E*)-3,4-dimethoxyphenyl enones were correlated with Hammett substituent constants (σ , σ^+ , σ_I , σ_R) [25, 29-32] and *F* and *R* parameters [33] using single and multi-linear regression analysis. 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 absorption maximum of the unsubstituted system.

The statistical analysis results were presented in **Table 3**. From the Table 3, it is evident that the UV absorption maximum λ_{max} (nm) values of all substituted it is evident that the UV absorption maximum λ_{max} (nm) values of all α , β -unsaturated ketones, except that with the 4-NO₂ substituent have shown satisfactory correlations with Hammett substituent constant viz., σ ($r = 0.969$). When the substituent 4-NO₂ that has been given exception is included in regression it reduces the correlations considerably.

Table 3. Results of statistical analysis of UV absorption maxima (λ_{max} , nm), IR frequencies (ν , cm^{-1}) and NMR chemical shifts (δ , ppm) of substituted (*E*)-3,4-dimethoxyphenylprop-2-en-1-ones. with Hammett substituent constants (σ , σ^+ , σ_I & σ_R) and *F* and *R* parameters.

Freq.	Constt.	<i>r</i>	<i>I</i>	ρ	<i>s</i>	<i>n</i>	Correlated derivatives
λ_{max}	σ	0.969	322.74	-28.65	11.26	8	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃
	σ^+	0.871	320.99	-22.49	9.37	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4-NO ₂
	σ_I	0.859	330.22	-34.37	12.10	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4-NO ₂
	σ_R	0.807	316.58	-4.77	14.97	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4-NO ₂
	<i>F</i>	0.752	328.65	-26.65	12.74	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4-NO ₂
	<i>R</i>	0.811	315.58	-6.12	14.91	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4-NO ₂
νCO_{s-cis}	σ	0.743	1651.44	3.18	2.21	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.739	1651.72	1.90	2.25	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.928	1651.01	2.68	2.35	7	3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-OCH ₃ , 4NO ₂
	σ_R	0.744	1652.95	4.69	2.19	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	<i>F</i>	0.817	1651.42	1.40	2.41	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	<i>R</i>	0.738	1652.90	3.34	2.26	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
$\nu\text{CO}_{s-trans}$	σ	0.708	1593.81	-2.73	10.59	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.702	1593.26	0.46	10.63	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.843	1599.89	-17.79	9.59	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.944	1597.44	20.32	9.52	7	H, 3-Br, 4-Br, 2-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	<i>F</i>	0.745	1600.13	-16.33	9.46	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	<i>R</i>	0.939	1597.41	15.03	9.76	7	H, 3-Br, 4-Br, 2-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
νCH_{ip}	σ	0.836	1156.97	-9.39	7.87	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.733	1156.14	-5.54	7.98	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.708	1156.37	-2.82	8.44	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂

	σ_R	0.757	1151.11	-20.84	6.93	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.711	1154.02	3.16	8.42	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.852	1151.04	-15.85	7.19	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
vCH_{op}	σ	0.757	785.25	-38.35	17.89	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.766	782.33	-28.48	16.43	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.722	785.71	-19.39	21.37	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.853	768.32	-50.63	18.50	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.709	781.46	-6.98	21.85	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.755	766.34	-43.59	18.21	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
vCH=CH_{op}	σ	0.852	1020.96	-4.27	2.31	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.758	1020.68	-3.11	2.19	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.731	1021.44	-3.31	2.57	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.933	1019.43	-3.89	2.56	7	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-CH ₃ , 4-NO ₂
	F	0.733	1021.49	-3.06	2.55	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.734	1019.32	-3.33	2.55	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
vC=C_{op}	σ	0.960	545.68	67.39	28.36	7	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-OCH ₃ , 4NO ₂
	σ^+	0.763	550.86	44.88	27.89	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.948	532.23	68.33	31.50	7	3-Br, 4-Br, 3-Cl, 2-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.729	566.59	45.25	34.53	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.932	540.95	39.58	34.13	7	3-Br, 4-Br, 3-Cl, 2-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.829	567.70	37.84	34.50	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
δH_α	σ	0.729	7.55	0.08	0.09	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.958	7.55	0.11	0.07	7	H, 3-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃

	σ_I	0.718	7.54	0.07	0.09	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.702	7.57	0.01	0.09	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.717	7.54	0.06	0.09	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.804	7.57	0.01	0.09	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
δH_β	σ	0.956	7.79	-0.11	0.06	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.829	7.78	-0.04	0.06	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.741	7.82	-0.10	0.06	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.862	7.74	-0.18	0.05	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.714	7.79	-0.03	0.07	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.862	7.74	-0.14	0.05	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
δCO	σ	0.850	189.28	5.80	3.30	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.846	189.79	3.45	3.39	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.840	188.09	5.96	3.50	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.850	191.97	8.29	3.30	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.823	189.02	3.05	3.72	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.846	192.01	6.32	3.39	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
δCa	σ	0.835	122.94	1.16	1.00	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ^+	0.832	123.03	0.74	1.00	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.845	122.45	1.89	0.95	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.830	122.86	-1.41	1.02	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.850	122.39	1.81	0.93	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.726	122.87	-1.02	1.03	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
$\delta C\beta$	σ	0.934	144.00	-2.75	2.42	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂

	σ^+	0.908	143.59	-0.41	2.57	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_I	0.821	144.30	-2.11	2.52	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	σ_R	0.857	142.24	-6.34	2.12	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	F	0.906	143.28	0.59	2.58	8	H, 3-Br, 4-Br, 3-Cl, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂
	R	0.856	142.12	-5.17	2.13	9	H, 3-Br, 4-Br, 3-Cl, 2-F, 4-F, 4-CH ₃ , 4-OCH ₃ , 4NO ₂

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

The UV absorption maximum λ_{max} (nm) values of all α , β -unsaturated ketone compounds have shown poor correlations ($r < 0.900$) with the remaining Hammett substituent constants and F and R parameters. This is attributed to the weak polar, inductive, field and resonance effects of the substituents for predicting the reactivity on the UV absorption through resonance as per the conjugative structure as shown in **Figure 1**.

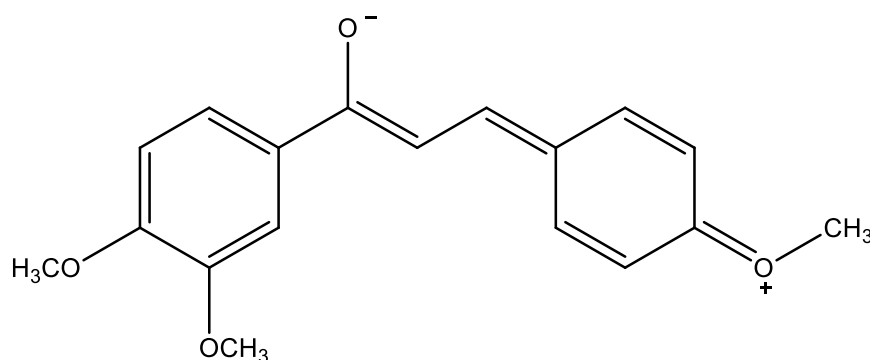


Figure 1. Resonance conjugative structure

All the correlations have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to UV absorption maximum λ_{max} (nm) values in all substituted (*E*)-3,4-dimethoxyphenyl enones. Since most of the single parameter correlations failed ($r < 0.900$) with Hammett constants σ , σ^+ , σ_R and *F* & *R* parameters, it is decided to go for multi regression analysis. While seeking the multi regression analysis, satisfactory correlations (good) are observed as shown in the following equations (2) and (3).

$$\lambda_{max}(\text{nm}) = 328.592(\pm 8.722) - 35.815(\pm 11.931) \sigma_I - 10.701(\pm 3.961) \sigma_R$$

($R = 0.961$, $n = 9$, $P > 90\%$) ... (2)

$$\lambda_{max}(\text{nm}) = 326.273(\pm 8.132) - 34.092(\pm 11.294) F - 20.197(\pm 6.30) R$$

($R = 0.963$, $n = 9$, $P > 90\%$) ... (3)

3.2. IR spectral study

The carbonyl stretching frequencies (cm^{-1}) of (*E*)-3,4-dimethoxyphenyl enones which exists as *s-cis* and *s-trans* conformers are shown in **Figure 2**. The IR frequency values are

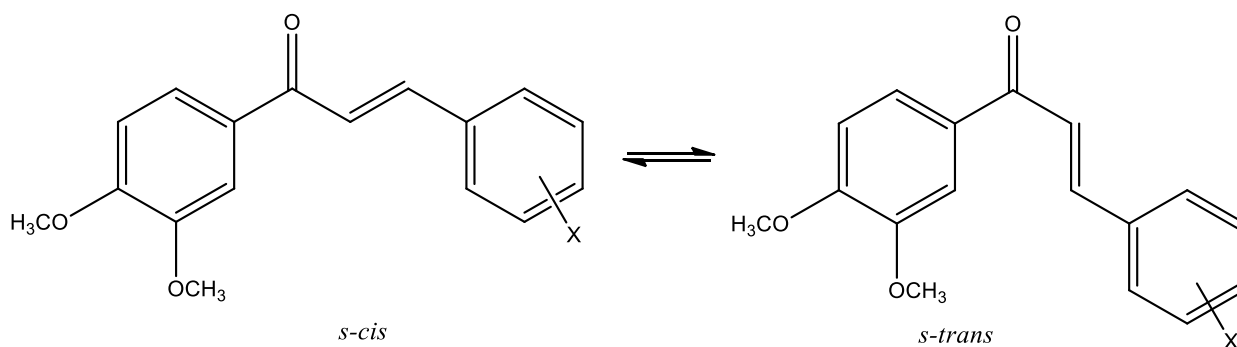


Figure 2. The *s-cis* and *s-trans* conformers of (*E*)-3,4-dimethoxyphenyl enones. presented in Table-2. The IR frequency values are correlated with Hammett substituent constants (σ , σ^+ , σ_I , σ_R) [25, 29, 30] and Swain-Lupton's parameters (*F*&*R*) [33]. While seeking Hammett correlation involving group frequencies, the form of the Hammett equation employed is

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

Where ν_0 is the carbonyl frequencies of unsubstituted system.

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

The statistical analysis results of infrared frequencies of $\nu\text{CO}_{s\text{-cis}}$ (cm^{-1}) of all substituted (*E*)-3,4-dimethoxyphenyl enones were presented in Table 3. It is evident that the IR frequency $\nu\text{CO}_{s\text{-cis}}$ (cm^{-1}) values of all (*E*)-3,4-dimethoxyphenyl enones, except those with the H(partent) and 4- CH_3 substituents have shown satisfactory correlations with Hammett substituent constant viz., σ_I ($r = 0.928$). When the substituents that have been given exception are included in regression, they reduce the correlations considerably.

The IR frequency $\nu\text{CO}_{s\text{-cis}}$ (cm^{-1}) values of all (*E*)-3,4-dimethoxyphenyl enones have shown poor correlations ($r < 0.900$) with the remaining Hammett substituent constants and *F* and *R* parameters. This is attributed to the weak polar, inductive, field and resonance effects of the substituents for predicting the reactivity on the IR frequency through resonance as per the conjugative structure as shown in **Figure 1**.

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

From Table-3, it is evident that the IR frequency $\nu\text{CO}_{s\text{-trans}}$ (cm^{-1}) values of all α,β -unsaturated ketone compounds, except those with the 3-Cl and 4-F substituents have shown satisfactory correlations with Hammett substituent constant viz., σ_R ($r = 0.944$) and *R* ($r = 0.939$) parameter. When the substituents that have been given exception are included in regression, they reduce the correlations considerably. This is due to the reasons stated earlier and associated with the resonance-conjugative structure as shown in Fig. 1. All the correlations except with σ^+ , σ_R and *R* parameter have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to IR frequency $\nu\text{CO}_{s\text{-trans}}$ (cm^{-1}) values in all α,β -unsaturated ketone compounds.

3.2.3. IR Spectral Correlation of νCH_{ip} νCH_{op} and (cm^{-1})

The IR frequency νCH_{ip} and νCH_{op} (cm^{-1}) values of all substituted (*E*)-3,4-dimethoxyphenyl enones shown poor correlations ($r < 0.900$) with all Hammett substituent

constants and F and R parameters. All the correlations except with F parameter have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to IR frequency of νCH_{ip} and νCH_{op} (cm^{-1}) values in all α,β -unsaturated ketones

3.2.4. IR Spectral Correlation of $\nu\text{CH}=\text{CH}_{OP}$ (cm^{-1})

The IR frequency $\nu\text{CH}=\text{CH}_{OP}$ (cm^{-1}) values of all (*E*)-3,4-dimethoxyphenyl enones except those with the 4-F and 4-OCH₃ substituents have shown satisfactory correlations with Hammett substituent constant viz., σ_R ($r = 0.933$). When the substituents that have been given exception are included in regression, they reduce the correlations considerably. These ketones have shown poor correlations ($r < 0.900$) with the remaining Hammett substituent constants and F and R parameters. The failure in correlation was due to the reason stated earlier. All the correlations have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to IR frequency $\nu\text{CH}=\text{CH}_{op}$ (cm^{-1}) values in all α,β -unsaturated ketones.

3.2.5. IR Spectral Correlation of $\nu\text{C}=\text{C}_{OP}$ (cm^{-1})

The IR frequency $\nu\text{C}=\text{C}_{OP}$ (cm^{-1}) values of all substituted (*E*)-3,4-dimethoxyphenyl enones except those with the 4-F and 4-CH₃ substituents have shown satisfactory correlations with Hammett substituent constant viz., σ ($r = 0.960$). The Hammett σ_I constant and F parameters showed satisfactory correlation σ_I ($r = 0.948$) and F ($r = 0.932$) except H(parent) and 4-F substituents. When the substituents that have been given exception are included in regression, they reduce the correlations considerably. 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 α, β -unsaturated ketones.

Most of the single regression analyses have shown poor correlation, it is decided to go for multi-regression analyses. The multi-regression produced satisfactory correlations (good) with Hammett substituent constants (σ , σ^+ , σ_I , σ_R) and F and R parameters [32,33]. The multi correlation equations are given in (5)-(16).

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1}) = 1651.814(\pm 1.481) + 3.385(\pm 3.216)\sigma_I + 5.257(\pm 3.561)\sigma_R$$

...(5)

$$(R = 0.956, n = 9, P > 95\%)$$

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1}) = 1651.959(\pm 1.467) + 3.104(\pm 1.121)F + 4.619(\pm 1.302)R$$

...(6)

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

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1}) = 1602.607(\pm 6.383) - 15.397(\pm 5.142)\sigma_I + 17.774(\pm 5.542)\sigma_R$$

...(7)

$$(R = 0.957, n = 9, P > 95\%)$$

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1}) = 1601.289(\pm 6.381) - 12.729(\pm 4.569)F + 9.779(\pm 3.359)R$$

...(8)

$$(R = 0.951, n = 9, P > 90\%)$$

$$\nu\text{CH}_{ip}(\text{cm}^{-1}) = 1153.051(\pm 4.988) - 5.761(\pm 2.826)\sigma_I - 21.794(\pm 7.246)\sigma_R$$

...(9)

$$(R = 0.959, n = 9, P > 90\%)$$

$$\nu\text{CH}_{ip}(\text{cm}^{-1}) = 1152.001(\pm 5.002) - 3.168(\pm 1.039)F - 17.160(\pm 5.279)R$$

...(10)

$$(R = 0.953, n = 9, P > 90\%)$$

$$\nu\text{CH}_{op}(\text{cm}^{-1}) = 777.318(\pm 12.655) - 26.838(\pm 8.964)\sigma_I - 55.077(\pm 18.413)\sigma_R \quad \dots(11)$$

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

$$\nu\text{CH}_{op}(\text{cm}^{-1}) = 775.021(\pm 11.631) - 27.187(\pm 9.072)F - 54.819(\pm 18.372)R$$

$$\dots(12)$$

$$(R = 0.965, n = 9, P > 95\%)$$

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1}) = 1020.751(\pm 1.731) - 3.926(\pm 1.758)\sigma_I - 4.548(\pm 1.615)\sigma_R$$

$$\dots(13)$$

$$(R = 0.959, n = 9, P > 90\%)$$

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1}) = 1020.862(\pm 1.494) - 5.065(\pm 1.188)F - 5.425(\pm 1.838)R$$

$$\dots(14)$$

$$(R = 0.961, n = 9, P > 90\%)$$

$$\nu\text{C}=\text{C}_{op}(\text{cm}^{-1}) = 541.053(\pm 21.006) + 76.156(\pm 25.583)\sigma_I + 57.866(\pm 19.483)\sigma_R$$

$$\dots(15)$$

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

$$\nu\text{C}=\text{C}_{op}(\text{cm}^{-1}) = 548.462(\pm 20.897) + 63.140(\pm 21.460)F + 63.907(\pm 21.209)R$$

$$\dots(16)$$

$$(R = 0.956, n = 9, P > 90\%)$$

3.3. NMR Spectral study

In Nuclear Magnetic Resonance spectra, the proton and the carbon chemical shifts (δ) depends on the electronic environment of the nuclei concerned. The assigned proton and carbon chemical shifts (ppm) have been correlated with reactivity parameters using Hammett equation in the form of

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

Where δ_0 is the chemical shift of unsubstituted system.

3.3.1. ^1H NMR Spectral correlation

3.3.1.1. ^1H NMR Spectral Correlations of H_α (ppm)

The assigned H_α chemical shift (δ , ppm) values of all substituted (*E*)-3,4-dimethoxyphenyl enones except those with the 4-Br and 4- NO_2 substituents have shown satisfactory correlations with Hammett substituent constant viz., σ^+ ($r = 0.958$). When the substituents that have been given exception are included in regression, they reduce the correlations considerably. All the correlations have shown positive ρ values. This indicates the operation of normal substituent effect operates in all systems. The remaining Hammett substituent constants and *F* and *R* parameters have shown poor correlations ($r < 0.900$). This is attributed to the weak of polar, inductive, field and resonance effects of the substituents for predicting the reactivity on the ^1H NMR chemical shift through resonance as per the conjugative structure as shown in **Figure 1**.

3.3.1.2. ^1H NMR Spectral Correlations of H_β (ppm)

The assigned H_β chemical shifts (δ , ppm) values of all are correlated with Hammett constants (σ , σ^+ , σ_I , σ_R) and *F* and *R* parameters, except that with the 2-F substituent have shown satisfactory correlations with Hammett substituent constant viz., σ ($r = 0.956$). When

the substituent that has been given exception is included in regression it reduces the correlations considerably. Remaining Hammett substituent constants and F and R parameters. have shown poor correlations ($r < 0.900$). This is due to reasons stated earlier. All the correlations have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to ^1H NMR chemical shift $\delta\text{H}_\beta(\text{ppm})$ values in all α , β -unsaturated ketones.

Some of the single regression analyses have shown poor correlations with Hammett substituent constants (σ , σ^+ , σ_I , σ_R) and Swain-Lupton's parameters [33]. It is decided to go for multi-regression, the multi-regression analysis produced satisfactory correlations (good) with the chemical shifts of (δ , ppm) H_α and H_β . The multi-correlation equations are given in (18)-(21).

$$\delta\text{H}_\alpha(\text{ppm}) = 7.587(\pm 0.057) + 0.149(\pm 0.077)\sigma_I - 0.115(\pm 0.153)\sigma_R \quad \dots(18)$$

$$(R = 0.963, n = 12, P > 90\%)$$

$$\delta\text{H}_\alpha(\text{ppm}) = 7.547(\pm 0.066) + 0.073(\pm 0.141)F + 0.044(\pm 0.149)R \quad \dots(19)$$

$$(R = 0.921, n = 12, P > 90\%)$$

$$\delta\text{H}_\beta(\text{ppm}) = 7.786(\pm 0.029) - 0.133(\pm 0.063)\sigma_I - 0.201(\pm 0.070)\sigma_R \quad \dots(20)$$

$$(R = 0.980, n = 12, P > 90\%)$$

$$\delta\text{H}_\beta(\text{ppm}) = 7.768(\pm 0.032) - 0.097(\pm 0.068)F - 0.185(\pm 0.072)R \quad \dots(21)$$

$$(R = 0.972, n = 12, P > 90\%)$$

3.3.2. ^{13}C NMR spectral correlation

3.3.2.1. ^{13}C NMR spectral correlation of δCO carbon

From Table-3, it is evident that the ^{13}C NMR chemical shift $\delta\text{CO}(\text{ppm})$ values of all (*E*)-3,4-dimethoxyphenyl enones have shown poor correlations ($r < 0.900$) with all Hammett substituent constants and F and R parameters. The failure in correlations was already stated the reasons also associated with the resonance-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 ^{13}C NMR chemical shift $\delta\text{CO}(\text{ppm})$ values in all α , β -unsaturated ketones.

3.3.2.2. ^{13}C NMR spectral correlation of δC_α carbon

The assigned C_α chemical shifts (δ , ppm) of all substituted (*E*)-3,4-dimethoxyphenyl enones have shown poor correlations ($r < 0.900$) with all Hammett substituent constants (σ , σ^+ , σ_I , σ_R) and F and R parameters. All the correlations (except σ_R and R parameter) have shown positive ρ values. This indicates the operation of normal substituent effect with respect to C_α chemical shifts (δ , ppm) values in all substituted (*E*)-3,4-dimethoxyphenyl enones:

3.3.2.3. ^{13}C NMR spectral correlation of δC_β carbon

The assigned C_β chemical shifts (δ , ppm) of all substituted (*E*)-3,4-dimethoxyphenyl enones except that with the 2-F substituent have shown satisfactory correlations with Hammett substituent constants viz., σ ($r = 0.934$), σ^+ ($r = 0.908$) and F ($r = 0.906$) parameter. When the substituent that has been given exception is included in regression it reduces the correlations considerably. Remaining Hammett substituent constants and R parameter. poor correlations ($r < 0.900$) with C_β chemical shifts (δ , ppm). All the correlations except with F

parameter have shown negative ρ values. This indicates the operation of reverse substituent effect with respect to ^{13}C NMR chemical shift $\delta\text{C}_\beta(\text{ppm})$ values in all α,β -unsaturated ketones.

Some of the single regression analyses have shown poor correlations with Hammett substituent (σ , σ^+ , σ_I , σ_R) constants and Swain-Lupton's parameters [31-33]. It is decided to go for multi-regression, the multi-regression analyses produced satisfactory correlations (good) with the chemical shifts of (δ , ppm) C_α , C_β and CO. The multi correlation equations are given in (22)-(27).

$$\delta\text{CO}(\text{ppm}) = 189.452(\pm 2.013) + 7.242(\pm 2.370)\sigma_I + 9.488(\pm 3.339)\sigma_R \quad \dots(22)$$

$$(R = 0.906, n = 9, P > 90\%)$$

$$\delta\text{CO}(\text{ppm}) = 190.074(\pm 2.034) + 6.352(\pm 2.325)F + 8.952(\pm 2.894)R \quad \dots(23)$$

$$(R = 0.906, n = 9, P > 90\%)$$

$$\delta\text{C}_\alpha(\text{ppm}) = 122.279 (\pm 0.676) + 1.737(\pm 0.569)\sigma_I - 1.120(\pm 0.362)\sigma_R \quad \dots(24)$$

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

$$\delta\text{C}_\alpha(\text{ppm}) = 122.354(\pm 0.646) + 1.691(\pm 0.572)F - 0.324(\pm 0.192)R \quad \dots(25)$$

$$(R = 0.950, n = 9, P > 95\%)$$

$$\delta\text{C}_\beta(\text{ppm}) = 143.261(\pm 1.452) - 3.029(1.010)\sigma_I - 6.842(\pm 2.291)\sigma_R \quad \dots(26)$$

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

$$\delta\text{C}_\beta(\text{ppm}) = 142.598(\pm 1.465) - 1.551(\pm 0.516)F - 5.813(\pm 1.837)R \quad \dots(27)$$

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

3.4. Antimicrobial activity

3.4.1. Antibacterial sensitivity assay

The antibacterial activities of all synthesized substituted (*E*)-3,4-dimethoxyphenyl enones have been studied against three gram positive and two gram negative pathogenic strains such as *Bacillus subtilis*, *Micrococcus luteus*, *Staphylococcus aureus*, *Escherichia coli* and *Pseudomonas aeruginosa* have been studied by Kirby-Bauer method [34]. Ampicillin was used as standard. The antibacterial screening effect of substituted *E*-3,4-dimethoxyphenyl enones is shown in **Figure 3** (Plates 1–10). The measured zone of inhibition values is given in **Table 4** and the corresponding clustered column chart is shown in **Figure 4**. Analysis of the zone of inhibition (mm) values reveals that the eight α , β -unsaturated ketone compounds with H(parent), 3-Br, 4-Br, 2-F, 4-F, 4-CH₃, 4-OCH₃ and 4-NO₂ substituents have shown moderate antibacterial activity against *Bacillus subtilis*. All enones shown moderate activity against *Micrococcus luteus* strain. The six α , β -unsaturated ketone compounds with H(parent), 3-Br, 2-F, 4-F, 4-CH₃ and 4-OCH₃ substituents in these ketones have shown moderate antibacterial activity against *Staphylococcus aureus*. The five α , β -unsaturated ketones with 3-Cl, 2-F, 4-CH₃, 4-OCH₃ and 4-NO₂ substituents have shown moderate antibacterial activity against *Escherichia coli*. The α , β -unsaturated ketone compound only with 4-Br substituent has shown good antibacterial activity against *Pseudomonas aeruginosa*. Remaining enones have shown poor antibacterial activity against their respective stains.

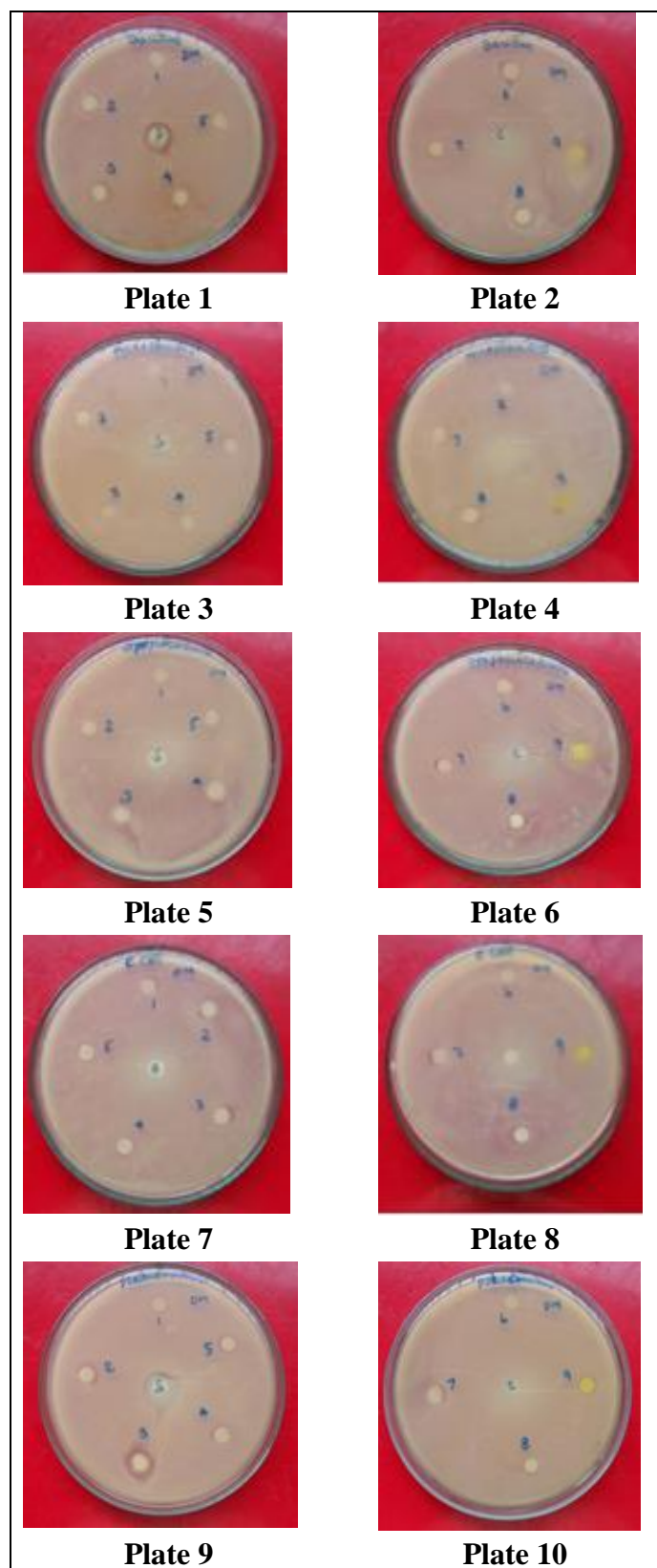
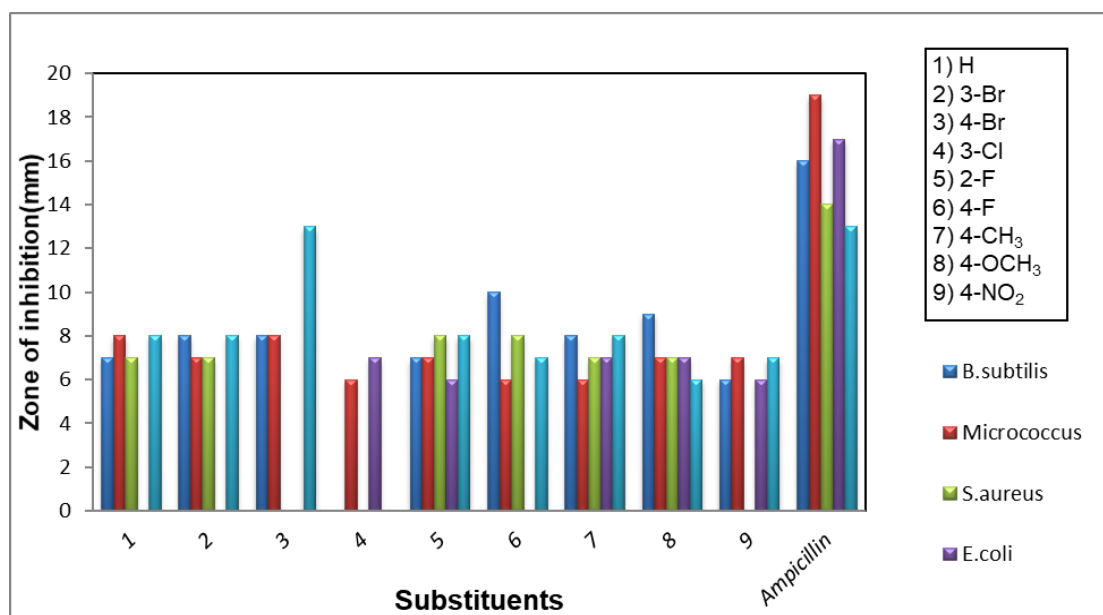


Figure 3. Antibacterial activity of substituted (*E*)-3,4-dimethoxyphenyl enones(petri plates).

Table 4. Zone of inhibition(mm) values of antibacterial activities of substituted (*E*)-3,4-dimethoxyphenyl enones.

Entry	Substituent	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>
1	H	7	8	7	-	8
2	3-Br	8	7	7	-	8
3	4-Br	8	8	-	-	13
4	3-Cl	-	6	-	7	-
5	2-F	7	7	8	6	8
6	4-F	10	6	8	-	7
7	4-CH ₃	8	6	7	7	8
8	4-OCH ₃	9	7	7	7	6
9	4-NO ₂	6	7	-	6	7
Standard	Ampicillin	16	19	14	17	13
Control	DMSO	-	-	-	-	-

**Figure 4.** Antibacterial activity of substituted (*E*)-3,4-dimethoxyphenyl enones (clustered column chart)

3.4.2. Antifungal sensitivity assay

The antifungal activities of all synthesized (*E*)-3,4-dimethoxyphenyl enones have been studied against two fungal species namely *Aspergillus niger*, and *Trichoderma species*. The disc diffusion technique has been followed using the Kirby–Bauer method [34], at a concentration of 250 µg/mL and ciprofloxacin was used as standard. The antifungal screening effect of prepared substituted (*E*)-3,4-dimethoxyphenyl enones are shown in **Figure 5**. (Plates 11–14). The measured zone of inhibition values is given in **Table 5** and the

corresponding Clustered column chart is shown in **Figure 6**. Analysis of the zone of inhibition(mm) values reveals that the five α , β -unsaturated ketone compounds with H(parent), 3-Br, 3-Cl, 2-F, 4-F and 4-OCH₃ substituents have shown moderate antifungal activity against *Aspergillus niger*. Parent H and 3-Br substituents have shown good and 4-Br, 3-Cl, 2-F, 4-CH₃ and 4-NO₂ substituents have shown moderate antifungal activity against *Trichoderma species*. The remaining α , β -unsaturated ketone compounds have shown poor antifungal activity against their stains.

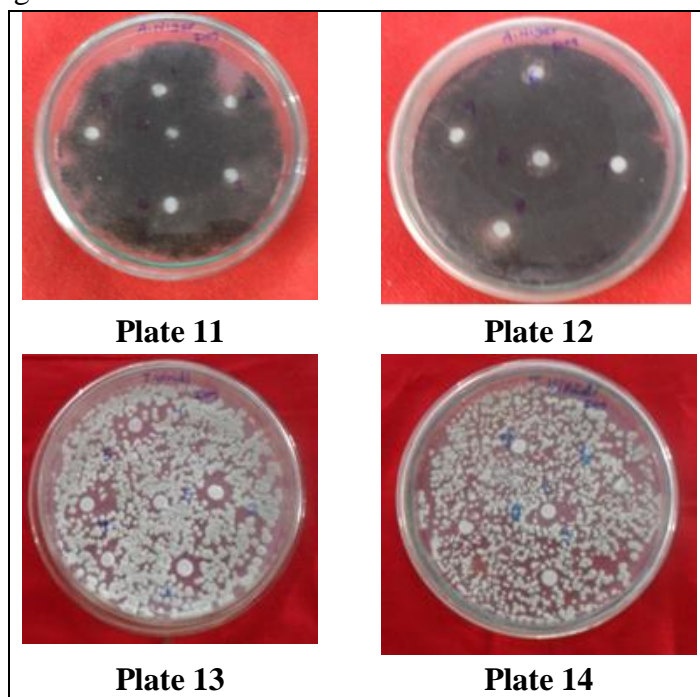


Figure 5. Antifungal activity of substituted (*E*)-3,4-dimethoxyphenyl enones (petri plates).

Table 5. Zone of inhibition (mm) values of antifungal activities of substituted (*E*)-3,4-dimethoxyphenyl enones.

Entry	Substituent	Zone of inhibition(mm)	
		<i>A. niger</i>	<i>T. viride</i>
1	H	7	10
2	3-Br	7	10
3	4-Br	-	9
4	3-Cl	8	7
5	2-F	7	8
6	4-F	-	-
7	4-CH ₃	-	7
8	4-OCH ₃	8	-
9	4-NO ₂	-	7
Standard	Miconazole	14	13
Control	DMSO	-	-

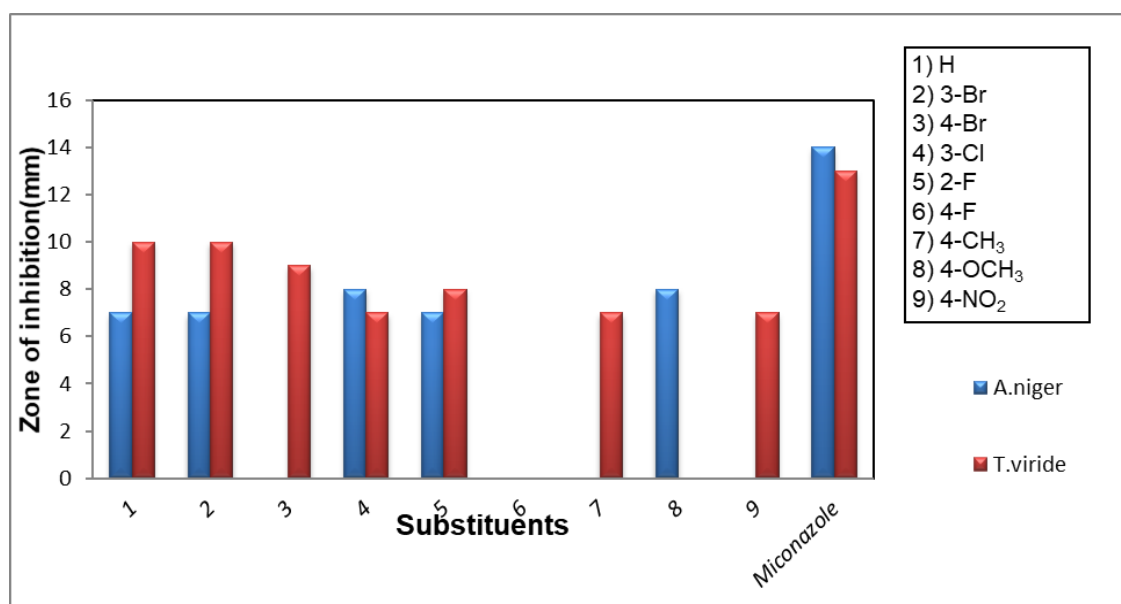


Figure 6. Antifungal activity of substituted (*E*)-3,4-dimethoxyphenyl enones (clustered column chart)

4. Conclusions

About nine numbers of substituted (*E*)-3,4-dimethoxyphenyl enones have been synthesized by ultrasound assisted cross-aldol condensation of 3,4-diethoxy acetophenone with various substituted benzaldehydes. The structure of all ketones has been confirmed by their physical constants, UV, IR and NMR spectral values. These spectral data have been correlated with Hammett substituent constants (σ , σ^+ , σ_I , σ_R), *F* and *R* parameters. In UV spectral analysis, a satisfactory correlation with Hammett substituent constant viz., σ ($r = 0.969$) was observed except 4-NO₂ substituent. The $\nu_{CO_{s-ciss}}$ (cm^{-1}) values of all α,β -unsaturated ketones shown satisfactory correlations with Hammett substituent constant viz., σ_I ($r = 0.928$) except H(parent) and 4-CH₃ substituents. The $\nu_{CO_{s-trans}}$ (cm^{-1}) values of all α,β -unsaturated ketones shown satisfactory correlations σ_R ($r = 0.944$) and *R* ($r = 0.939$) with Hammett substituent except 3-Cl and 4-F substituents. All correlations of $\nu_{CH_{ip}}$ and $\nu_{CH_{op}}$ (cm^{-1}) (*E*)-3,4-dimethoxyphenyl enones shown poor correlations ($r < 0.900$) with Hammett substituent constants and *F* and *R* parameters. The $\nu_{CH=CH_{OP}}$ (cm^{-1}) frequencies shown satisfactory correlations with Hammett substituent constant viz., σ_R ($r = 0.933$). except with the 4-F and 4-OCH₃ substituents. The $\nu_{C=C_{OP}}$ (cm^{-1}) frequencies correlated satisfactorily with Hammett substituent constant viz., σ ($r = 0.960$) except 4-F and 4-CH₃ substituents have shown satisfactory correlations. Similarly, the Hammett σ_I constant and *F* parameters showed satisfactory correlation σ_I ($r = 0.948$) and *F* ($r = 0.932$) except H(parent) and 4-F substituents. The H_α chemical shifts (δ , ppm) shown satisfactory correlations with Hammett substituent constant viz., σ^+ ($r = 0.958$) except those with the 4-Br and 4-NO₂ substituents. The H_β chemical shifts (δ , ppm) satisfactory correlated with Hammett constant σ ($r = 0.956$) except 2-F substituent. In ¹³C NMR spectral correlations, the chemical shifts (ppm) of CO and C _{α} carbons were failed in correlations. The C _{β} chemical shifts (δ , ppm) correlated satisfactory

with with Hammett substituent constants viz., σ ($r = 0.934$), σ^+ ($r = 0.908$) and F ($r = 0.906$) parameter except 2-F substituent. All multi-regressions shows satisfactory correlations. All ketons shows satisfactory, moderate and good antibacterial and antifungal activities against their stains.

Acknowledgments

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