Spectral LFER studies on some sydnone chalcones

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ABSTRACT. A series containing ten (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates were prepared and examined their purities by literature method. The infrared and NMR spectral data were assigned and correlated with Hammett substituent constants and Swain-Lupton's constants using single and multi-regression analysis. From the results of statistical analyses the effects of substituents on the spectral data have been discussed.

1. INTRODUCTION

Sydnone are five membered mesoionic dipolar compounds [1]. With reactivity and stability they are fairly different compounds from other aromatics [2]. Sydnones plays on important role in medicinal, heterocyclic and theoretical chemistry [3]. These compounds used as key intermediates for synthesis of organic compounds and possess physiological potentials. They possess many biological activities such as antimicrobial[4], antiviral[5], anti-tumour[6], analgesic[7], anti-inflammatory[8], anthelmintic[9], free-radical scavenging[10], nitric oxide donor[11] and anti-cancer[12]. Sydnone chalcones also possess these properties. Spectroscopic data were useful for prediction of geometry and ground state equilibration of organic compounds[13]. From vibrational spectra the *s-cis* and *s-trans* conformations of carbonyl compounds were predicted[14]. The chemical shifts of NMR spectra were useful for prediction of geometry of compounds such as *E* or *Z* along with coupling constants[15]. Proton chemical shifts splitting patterns used for prediction of spatial arrangement of heterocyclic ring protons in cyclohexane and five membered pyrazolines[16]. Correlation analysis was used for studying reaction speeds, structural conformations of alkenes [17], alkynes [18], α,β -unsaturated aldehydes[19], ketones[20], ω -substituted ketones[21] and its esters, halo acyl bromides[22], ¹H pyrazoles [23] and its derivatives. Thirunarayanan and Manikandan have studied the dosage of drug analysis using correlation study[24]. Thirunarayanan et al., have studied the infrared and NMR spectral correlations of phenazine and quinoxaline derivatives [21, 22]. Mayavel et al., have studied the spectral correlation of some *E*-imines [23]. The Qsar and Qpr spectral correlation of some dihyroisoxazoles were reported by Thirunarayanan and Sathiyendiran [25]. Thirunarayanan and his co-workers have studied the effect of substituents on spectral data of some oxazine-2-amines[26]. The spectral correlation of infrared and carbon-13 NMR data of quinoxaline and phenazine derivatives were studied by Thirunaryanan et al. [27, 28]. Senbagam et al., have studied the effects of substituents on some substituted (*E*)-*N*-benzylidene-4*H*-1,2,4-triazol-4-amines[29]. Vijayakumar et al., have investigated the spectral correlation analysis on some (*E*)-2-benzylidenehydrazine carbothioamides[30]. The effect of substituents on some hydrazine derivatives were investigated by Rajarajan et al.,[31]. On the complete literature survey, the similar study was not reported with sydnone based chalcones. Hence, the authors have reported first time and taken efforts for the study of spectral correlation of the titled compounds by IR and NMR spectra.

2. EXPERIMENTAL

2.1. General

In this present investigations, chemicals used were purchased from Sigma-Aldrich Company Bangalore, India. Infrared spectra (KBr, 4000–400 cm^{-1}) were recorded on a Briker (Thermo Nicolet) Fourier transform spectrophotometer. The NMR spectra of all pyrazolines were recorded on a Bruker AV400 spectrometer operating at 400 MHz to record ^1H and 100 MHz for ^{13}C spectra in CDCl_3 solvent with TMS as internal standard.

2.2. Synthesis of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates

In this present study, the titled compounds were synthesised and characterized by literature method[32]. The general structure of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates are shown in Fig.1.

Fig. 1. The general structure of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates

3. RESULTS AND DISCUSSION

3.1. Correlation analysis with IR spectral data

Infrared spectra of synthesized (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates, the characteristic stretches (ν , cm^{-1}) of $\text{CO}_{s\text{-}cis}$, $s\text{-}trans$, $\text{CH}_{ip, op}$, $\text{CH}=\text{CH}_{op}$, $\text{C}=\text{C}_{op}$, NH , SO_2 , and CO_{syd} have been assigned and tabulated in Table 1. Using Hammett equation and single and multi-regression analysis[13-16, 20-31] of these data with Hammett substituent constants and Swain-Lupton's [33] parameters. In this correlation, the Hammett equation was taken in the form as(1).

Table 1. The infrared characteristics vibrations (ν , cm^{-1}) of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates

Entry	X	CO _{s-cis}	CO _{s-trans}	CH _{ip}	CH _{op}	CH=CH _{op}	C=C _{op}	NH	SO ₂	CO _{syd}
1	H	1618	1610	1175	763	1048	576	3315	1327	1756
2	3-Br	1628	1595	1176	767	1046	570	3322	1318	1758
3	2-Cl	1620	1594	1177	767	1046	570	3335	1320	1750
4	4-Cl	1621	1601	1174	765	1044	571	3536	1319	1754
5	4-F	1602	1631	1174	765	1045	572	3311	1322	1753
6	4-OH	1623	1594	1174	764	1044	572	3308	1310	1755
7	2-OCH ₃	1621	1593	1175	763	1044	572	3312	1324	1754
8	4-OCH ₃	1622	1595	1170	757	1043	569	3329	1316	1748
9	4-CH ₃	1648	1606	1168	758	1042	569	3308	1318	1752
10	4-NO ₂	1654	1608	1172	768	1053	578	3347	1328	1786

$$\nu = \nu_0 + \rho\sigma \quad (1)$$

where ν_0 is the unsubstituted system.

the obtained statistical results are tabulated in Table 2. From the Table 2, the CO_{s-cis} stretches (ν , cm^{-1}) gave satisfactory correlations with Hammett σ_I , σ_R , constants, F and R parameters positive ρ values excluding 4-CH₃ and 4-NO₂ substituents. This ρ value indicates that, the normal substituent effects operate in all systems. The Hammett σ and σ^+ constants produced poor correlation. The CO_{s-trans} stretches (ν , cm^{-1}) of the sydnone chalcones produced satisfactory correlation with Hammett σ , σ^+ , σ_R constants and R parameters excluding H, 2-Cl, and 2-OCH₃ substituents. The inductive and field components of the substituents produced poor correlations. The failure in correlation was the inability of prediction of effects of substituents on the stretches and attributed with the resonance-conjugative structure as illustrated in Fig. 2.

Fig. 2. The resonance-conjugative structure

Table 2. Results of statistical analysis of infrared vibrations (ν , cm^{-1}) of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
$\text{CO}_{s\text{-}cis}$	σ	0.728	1629.35	13.061	20.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.736	1652.35	9.572	19.68	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.905	1630.86	43.562	17.36	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃
	σ_R	0.900	1644.88	65.836	12.26	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.905	1646.36	47.262	12.76	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ ,
	R	0.900	1642.35	35.682	16.84	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
$\text{CO}_{s\text{-}trans}$	σ	0.906	1599.13	14.539	6.55	9	H, 3-Br, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.905	1600.00	8.439	7.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.804	1599.20	1.578	8.69	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.909	1607.42	30.856	4.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.800	1599.92	0.355	8.71	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.908	1607.25	24.854	4.68	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CH_{ip}	σ	0.906	1173.82	10.280	4.73	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 4-OCH ₃ , 4-NO ₂
	σ^+	0.906	1174.82	6.599	4.89	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 4-OCH ₃ , 4-NO ₂
	σ_I	0.917	1167.49	20.086	3.97	9	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.821	1175.57	5.140	6.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.902	1169.92	17.701	4.34	9	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.824	1175.93	5.257	6.22	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CH_{op}	σ	0.926	764.13	7.854	3.45	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.907	765.18	4.812	3.68	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.907	760.05	13.991	3.21	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.831	766.25	5.884	4.39	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.906	760.74	11.272	3.66	9	H, 3-Br, 2-Cl, 4-Cl, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.827	766.21	4.591	4.43	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
$\text{CH}=\text{CH}_{op}$	σ	0.907	1045.19	6.695	4.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.907	1048.88	8.885	4.17	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂

	σ_I	0.847	1043.27	6.572	2.93	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.906	1047.24	4.002	2.41	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃
	F	0.830	1047.63	5.171	3.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.906	1047.84	7.542	2.47	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃
$\text{C}=\text{C}_{op}$	σ	0.905	570.25	7.409	4.19	8	3-Br, 2-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.905	570.98	4.794	4.27	8	3-Br, 2-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.823	568.68	8.741	4.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.905	573.38	11.281	4.27	7	H, 3-Br, 2-Cl, 4-Cl, 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.827	568.60	5.546	4.90	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.905	573.29	8.643	4.41	7	H, 3-Br, 2-Cl, 4-Cl, 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
NH	σ	0.907	3321.03	27.485	9.78	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.906	3323.61	16.491	10.99	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.906	3309.27	38.483	11.33	9	H, 3-Br, 2-Cl, 4-Cl, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.905	3329.68	29.895	12.55	8	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-NO ₂
	F	0.843	3313.24	25.148	13.13	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.915	3330.85	27.462	12.11	8	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-NO ₂
SO_2	σ	0.833	1321.13	3.340	3.97	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.836	1321.15	2.656	3.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.811	1320.89	2.069	4.18	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.836	1322.28	6.187	3.92	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.811	1320.59	1.954	4.18	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.841	1323.16	5.944	3.82	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CO_{syd}	σ	0.907	1755.64	21.382	7.65	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.905	1757.52	11.630	9.12	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.904	1749.03	22.330	10.04	8	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-NO ₂
	σ_R	0.906	1763.85	29.361	8.72	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.841	1749.92	18.535	10.37	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.905	1763.71	22.830	9.16	9	H, 3-Br, 2-Cl, 4-Cl, 4-F, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂

r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents

The correlation of deformation modes of CH_{ip} (ν , cm^{-1}) of the synthesised sydnone chalcones gave satisfactory correlations with Hammett σ , σ^+ , σ_I constants and F parameters excluding H, 2-OCH₃ and 4-CH₃ substituents. The resonance components of the substituents were fail in correlation.

The correlation of deformation modes of CH_{op} (ν , cm^{-1}) of the synthesised sydnone chalcones gave satisfactory correlations with Hammett σ , σ^+ , σ_I constants and F parameters excluding 4-F and 4-OH substituents. Also here the resonance components of the substituents were fail in correlation.

The correlation of deformation modes of $\text{CH}=\text{CH}_{op}$ (ν , cm^{-1}) of the synthesised sydnone chalcones gave satisfactory correlations with Hammett σ , σ^+ , σ_R constants and R parameters excluding 4-NO₂ substituent. The inductive and field components of the substituents were fail in correlation.

The correlation of deformation modes of $\text{C}=\text{C}_{op}$ (ν , cm^{-1}) of the synthesised sydnone chalcones gave satisfactory correlations with Hammett σ , σ^+ , σ_R constants and R parameters excluding H, 4-F, 4-OH and 2-OCH₃ substituents. The inductive and field components of the substituents were fail in correlation.

The NH stretches (ν , cm^{-1}) of chalcones gave satisfactory correlation with Hammett substituent constants and R parameters excluding 4-F and 4-CH₃ substituents. Here, the field components of the substituents were fail in correlation.

The poor correlations obtained for the SO₂ stretches (ν , cm^{-1}) of chalcones with Hammett substituent constants, F and R parameters.

A satisfactory correlation was obtained for CO_{syd} (ν , cm^{-1}) of chalcones with Hammett substituent constants and R parameters. The field effect of the substituents were fail for production of correlation. The reason for failure in correlation was already stated and along with resonance-conjugation structure as illustrated in Fig. 2.

In single parameter infrared spectral correlations, some of the Hammett substituent constants, F and R parameters were fail for giving correlation coefficients. When these data are produced satisfactory correlations in multi-regression analysis with σ_I , σ_R and Swain-Lupton's constants[33]. The generated multi-regression analysis equations are given in (2-19).

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1}) = 1661.14 (\pm 5.453) + 43.603 (\pm 11.700) \sigma_I + 65.843 (\pm 11.277) \sigma_R \quad (2)$$

($R = 0.983$, $n=10$, $P > 95\%$)

$$\nu\text{CO}_{s-cis}(\text{cm}^{-1}) = 1660.04 (\pm 6.327) + 40.784 (\pm 13.298) F + 49.056 (\pm 11.336) R \quad (3)$$

($R = 0.990$, $n=10$, $P > 95\%$)

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1}) = 1606.83 (\pm 3.0517) + 1.749 (\pm 0.124) \sigma_I + 30.863 (\pm 6.314) \sigma_R \quad (4)$$

($R = 0.987$, $n=10$, $P > 95\%$)

$$\nu\text{CO}_{s-trans}(\text{cm}^{-1}) = 1606.45 (\pm 3.322) + 3.268 (\pm 0.691) F + 25.185 (\pm 5.953) R \quad (5)$$

($R = 0.990$, $n=10$, $P > 95\%$)

$$\nu\text{CH}_{ip}(\text{cm}^{-1}) = 1168.76 (\pm 2.737) + 20.085 (\pm 5.959) \sigma_I + 5.139 (\pm 5.749) \sigma_R \quad (6)$$

($R = 0.973$, $n=10$, $P > 95\%$)

$$\nu\text{CH}_{ip}(\text{cm}^{-1}) = 1169.79 (\pm 2.736) + 18.745 (\pm 5.780) F + 2.236 (\pm 4.903) R \quad (7)$$

($R = 0.979$, $n=10$, $P > 95\%$)

$$\nu\text{CH}_{op}(\text{cm}^{-1}) = 761.50 (\pm 2.109) + 13.995 (\pm 4.526) \sigma_I + 5.884 (\pm 2.314) \sigma_R \quad (8)$$

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

$$\nu\text{CH}_{op}(\text{cm}^{-1}) = 762.24 (\pm 2.334) + 12.107 (\pm 4.905) F + 5.814 (\pm 2.118) R \quad (9)$$

($R = 0.971$, $n=10$, $P > 95\%$)

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1}) = 1045.49 (\pm 1.406) + 6.574 (\pm 3.014) \sigma_I + 9.020 (\pm 2.910) \sigma_R \quad (10)$$

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

$$\nu\text{CH}=\text{CH}_{op}(\text{cm}^{-1}) = 1045.76 (\pm 1.364) + 6.352 (\pm 2.867) F + 8.207 (\pm 2.445) R \quad (11)$$

($R = 0.982$, $n=10$, $P > 95\%$)

$$\nu\text{C}=\text{C}_{op}(\text{cm}^{-1}) = 571.44 (\pm 2.988) + 5.740 (\pm 0.625) \sigma_I + 11.280 (\pm 5.210) \sigma_R \quad (12)$$

($R = 0.960$, $n=10$, $P > 95\%$)

$$\nu_{C=C_{op}}(\text{cm}^{-1}) = 571.03(\pm 2.931) + 6.895(\pm 1.625)F + 9.370(\pm 2.697)R \quad (13)$$

($R = 0.960$, $n=10$, $P > 95\%$)

$$\nu_{NH}(\text{cm}^{-1}) = 3316.65(\pm 6.331) + 38.429(\pm 13.888)\sigma_I + 29.893(\pm 13.098)\sigma_R \quad (14)$$

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

$$\nu_{NH}(\text{cm}^{-1}) = 3321.16(\pm 6.921) + 29.544(\pm 4.258)F + 30.554(\pm 5.368)R \quad (15)$$

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

$$\nu_{SO}(\text{cm}^{-1}) = 1322.12(\pm 2.875) + 2.068(\pm 6.169)\sigma_I + 6.180(\pm 1.325)\sigma_R \quad (16)$$

($R = 0.938$, $n=10$, $P > 90\%$)

$$\nu_{SO}(\text{cm}^{-1}) = 1322.17(\pm 2.706) + 12.895(\pm 5.685)F + 6.288(\pm 1.850)R \quad (17)$$

($R = 0.945$, $n=10$, $P > 90\%$)

$$\nu_{CO_{syd}}(\text{cm}^{-1}) = 1756.28(\pm 5.144) + 22.329(\pm 1.025)\sigma_I + 29.365(\pm 10.571)\sigma_R \quad (18)$$

($R = 0.979$, $n=10$, $P > 95\%$)

$$\nu_{CO_{syd}}(\text{cm}^{-1}) = 1756.44(\pm 5.256) + 22.154(\pm 6.358)F + 25.148(\pm 0.942)R \quad (19)$$

($R = 0.976$, $n=10$, $P > 90\%$)

3.2. NMR Spectral correlations

3.2.1. ^1H NMR spectral study

In the present study, the compounds chosen for evaluating the effects of substituents on the sydnone chalcones was shown in Fig. 1. The NMR spectra of synthesised sydnone chalcone were recorded in CDCl_3 solvent using TMS as internal standard. The Chemical shifts (δ , ppm) of vinyl protons, NH and methyl protons of synthesised sydnone chalcones were presented in Table 3. These chemical shifts(δ , ppm) have been correlated with Hammett substituent constants, F and R parameters using single and multi-linear regression analysis [13-16, 20-32]. In this correlation the Hammett equation was taken in the form as(20)

$$\delta = \rho\sigma + \delta_0 \quad (20)$$

where δ_0 is the frequency for the parent member of the series.

Table 3. The ^1H NMR chemical shifts (δ , ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates.

Entry	X	H_α	H_β	NH	CH_3
1	H	6.853	7.431	8.243	2.381
2	3-Br	6.781	7.452	8.217	2.343
3	2-Cl	6.281	7.603	9.213	2.317
4	4-Cl	7.411	6.413	9.413	2.372
5	4-F	7.613	8.171	9.571	2.345
6	4-OH	7.061	7.123	9.459	2.460
7	2-OCH ₃	7.071	7.172	9.381	2.361
8	4-OCH ₃	6.671	7.342	9.109	2.306
9	4-CH ₃	6.687	7.347	9.061	2.297
10	4-NO ₂	7.773	7.643	9.721	2.413

The results of statistical analysis of these proton chemical shifts of sydnone chalcones with Hammett substituent constants were presented in Table 4.

Table 4. Results of statistical analysis of ^1H NMR chemical shifts (δ , ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
H_α	σ	0.837	6.907	0.491	0.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.819	7.006	0.165	0.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.905	6.572	1.242	0.11	8	H, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.804	7.001	0.096	0.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.906	6.499	1.347	0.12	8	H, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.800	6.995	0.807	0.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
H_β	σ	0.907	7.372	0.408	0.12	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.908	7.414	0.279	0.12	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.834	7.792	0.292	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.907	7.542	0.626	0.13	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.813	7.358	0.104	0.13	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.908	7.568	0.573	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
NH	σ	0.801	9.130	0.140	0.54	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.809	9.132	0.084	0.54	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.904	8.723	1.088	0.48	9	H, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.828	8.989	0.639	0.52	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.905	8.174	1.181	0.46	8	2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.828	8.971	0.538	0.52	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CH_3	σ	0.817	2.358	0.014	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.805	2.359	0.047	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.820	2.344	0.441	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.809	2.364	0.024	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.820	2.344	0.042	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.826	2.358	0.041	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents							

From Table 4, the correlation of H_α chemical shifts (ppm) of sydnone chalcones gave satisfactory correlation coefficients with Hammett σ_I constant and F parameter excluding 3-Br and 2-Cl substituents. The remaining Hammett σ , σ^+ , σ_R constants and R parameters were failing in correlations.

A satisfactory correlation was obtained for H_β chemical shifts (ppm) with Hammett σ , σ^+ , σ_R constants and R parameters. The inductive and field components of the substituents were fail in correlations.

The Hammett σ_I constant and F parameters gave satisfactory correlation with the chemical shifts(ppm) of NH protons of the synthesised sydnone chalcones excluding 3-Br substituent. The Hammett σ , σ^+ , σ_R constants and R parameters gave poor correlations with NH proton chemical shifts(ppm) of sydnone chalcones,

The Hammett substituent constants, F and R parameters were fail in correlation for the methyl proton chemical shifts(ppm) of sydnone chalcones. The reason for the failure in correlation was already stated in earlier and associated with resonance-conjugated structure as shown in Fig. 2. In proton chemical shift correlations, all single regressions gave positive ρ values. This means that the normal substituent effect operates in all system.

In single parameter proton chemical shift correlations, some of them are failed. While seeking these in multi-regression analysis[33], they are worthwhile and produced satisfactory correlations. The generated multi-regression analysis equations are given in(21-28).

$$\delta\text{H}_\alpha(\text{ppm}) = 6.595(\pm 0.307) + 1.242(\pm 0.655)\sigma_I + 0.990(\pm 0.065)\sigma_R \quad (21)$$

($R = 0.958$, $n=10$, $P > 95\%$)

$$\delta\text{H}_\alpha(\text{ppm}) = 6.539(\pm 0.270) + 1.393(\pm 0.567)F + 0.153(\pm 0.045)R \quad (22)$$

($R = 0.968$, $n=10$, $P > 95\%$)

$$\delta\text{H}_\beta(\text{ppm}) = 7.447(\pm 0.081) + 0.292(\pm 0.174)\sigma_I + 0.620(\pm 0.124)\sigma_R \quad (23)$$

$$(R = 0.983, n=10, P > 95\%)$$

$$\delta H_{\beta}(\text{ppm}) = 7.505(\pm 0.073) + 0.192(\pm 0.012)F + 0.568(\pm 0.125)R \quad (24)$$

$$(R = 0.986, n=10, P > 95\%)$$

$$\delta \text{NH}(\text{ppm}) = 8.614(\pm 1.089) + 1.085(\pm 0.732)\sigma_1 + 0.630(\pm 0.074)\sigma_R \quad (25)$$

$$(R = 0.959, n=10, P > 95\%)$$

$$\delta \text{NH}(\text{ppm}) = 8.604(\pm 0.322) + 1.122(\pm 0.625)F + 0.427(\pm 0.025)R \quad (26)$$

$$(R = 0.958, n=10, P > 95\%)$$

$$\delta \text{CH}_3(\text{ppm}) = 2.349(\pm 0.036) + 0.042(\pm 0.002)\sigma_1 + 0.258(\pm 0.123)\sigma_R \quad (27)$$

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

$$\delta \text{CH}_3(\text{ppm}) = 2.344(\pm 0.037) + 0.042(\pm 0.007)F + 0.303(\pm 0.067)R \quad (28)$$

$$(R = 0.920, n=10, P > 90\%)$$

3.2.2. ^{13}C NMR spectral study

The ^{13}C NMR spectral chemical shifts(ppm) of synthesised sydnone chalcones are presented in Table 5. These data are correlated with Hammett substituent constants, F and R parameters using single and multi-linear regression analysis[13-16, 20-320]. The results of single parameter correlation analysis of ^{13}C NMR spectral chemical shifts(ppm) of synthesised sydnone chalcones are tabulated in Table 6. From Table 6, the correlation of $\delta \text{CO}(\text{ppm})$ of the chalcones gave satisfactory correlation coefficients with Hammett σ^+ , σ_1 constants and F parameters. The remaining Hammett σ , σ_R constants and R parameters fail in correlations. This is due to the inability of substituents effects already stated and associated with conjugative structure as shown in Fig. 2.

Table 5. The ^{13}C NMR chemical shifts (δ , ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates.

Entry	X	CO	C $_{\alpha}$	C $_{\beta}$	Ar-C-C $_{\beta}$	Ar-C-CO	Ar-C-NH	C-S	CO $_{\text{syd}}$	Ar-C-N $^+$	Ar-C-CH $_3$	CH $_3$
1	H	188.74	119.23	145.27	127.52	127.66	144.72	110.28	172.74	135.82	141.73	23.31
2	3-Br	188.69	119.24	140.38	127.54	127.28	144.36	110.34	174.13	135.71	141.28	22.52
3	2-Cl	189.06	119.23	145.64	128.65	127.28	144.21	111.34	174.89	136.06	141.36	22.33
4	4-Cl	188.85	120.13	145.37	128.35	127.14	144.28	110.21	175.24	135.68	141.31	22.87
5	4-F	189.41	120.03	145.26	128.63	127.24	144.31	110.27	175.93	135.51	141.48	21.36
6	4-OH	188.11	120.04	144.97	127.74	127.16	144.32	110.24	174.88	135.38	141.29	21.61
7	2-OCH $_3$	188.96	120.14	145.19	127.36	127.01	144.14	110.19	174.92	138.27	141.21	21.35
8	4-OCH $_3$	184.03	118.97	145.06	127.23	126.98	144.03	109.89	173.98	135.27	140.83	21.43
9	4-CH $_3$	184.95	119.72	145.17	128.54	127.20	144.19	110.14	174.25	135.72	140.98	22.06
10	4-NO $_2$	188.98	120.31	146.08	128.96	128.11	145.07	111.76	175.06	135.97	141.33	23.65

Table 6. Results of statistical analysis of ^{13}C NMR chemical shifts (δ , ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
CO	σ	0.848	188.62	0.673	0.48	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.906	188.70	0.883	0.43	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.906	188.16	1.430	0.43	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.801	188.65	0.022	0.35	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.900	188.165	1.345	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.878	188.751	0.330	0.54	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
C_α	σ	0.808	119.72	0.188	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.805	119.72	0.055	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.832	119.47	0.732	0.51	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.808	119.67	0.186	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.839	119.42	0.881	0.49	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.819	119.66	0.194	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
C_β	σ	0.956	145.30	0.777	0.14	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.927	145.38	0.524	0.14	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.906	145.04	0.881	0.26	8	3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-NO ₂
	σ_R	0.906	145.56	0.913	0.25	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.848	145.102	0.653	0.29	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.927	145.60	0.843	0.22	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
Ar-C- C_β	σ	0.902	128.06	0.657	0.64	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.912	128.01	0.640	0.62	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.892	127.95	0.912	1.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.901	127.85	0.265	0.65	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.906	127.69	0.658	0.68	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.904	127.68	0.394	0.69	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
Ar-C-CO	σ	0.908	127.32	0.764	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.908	127.39	0.490	0.21	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂

	σ_I	0.835	127.28	0.530	0.33	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.962	127.66	1.222	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.825	127.22	0.361	0.34	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.943	127.68	1.022	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
Ar-C-NH	σ	0.907	144.34	0.599	0.22	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.906	144.39	0.389	0.24	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.829	144.24	0.360	0.31	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.907	144.61	1.100	0.20	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.811	144.34	0.376	0.32	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.912	144.24	0.412	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CS	σ	0.907	110.41	1.201	0.41	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.917	110.53	1.811	0.40	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.857	109.95	1.438	0.51	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.854	110.80	1.375	0.52	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.843	110.05	1.133	0.55	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.857	110.84	1.233	0.51	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
CO _{hyd}	σ	0.815	174.88	0.375	0.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.810	174.65	0.171	0.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.907	173.68	2.717	0.65	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.837	174.25	2.140	0.85	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.907	173.56	2.874	0.57	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.835	174.25	2.112	0.86	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
Ar-C-N ⁺	σ	0.907	135.61	0.567	0.19	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.908	135.67	0.429	0.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.820	135.55	0.245	0.28	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.901	135.87	0.917	0.17	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.817	134.76	0.371	0.27	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.900	136.13	0.417	0.17	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
Ar-C-CH ₃	σ	0.906	141.37	0.525	0.24	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂

	σ^+	0.906	141.36	0.359	0.24	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.836	141.16	0.481	0.29	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.905	141.50	0.700	0.27	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-NO ₂
	F	0.835	141.74	0.439	0.30	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.905	141.52	0.600	0.26	8	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-NO ₂
CH ₃	σ	0.981	22.27	1.835	0.47	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ^+	0.982	22.45	1.221	0.49	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_I	0.828	22.00	1.040	0.83	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	σ_R	0.908	23.06	2.365	0.49	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	F	0.824	22.05	0.825	0.84	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
	R	0.905	23.12	2.462	0.47	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH ₃ , 4-OCH ₃ , 4-CH ₃ , 4-NO ₂
r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents							

The vinyl alpha carbon chemical shifts(ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters were fail for production of satisfactory or good correlations.

The vinyl beta carbon chemical shifts(ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett substituent constants and R parameters produced satisfactory correlations excluding 4-CH₃ substituent.

A satisfactory correlation coefficients obtained for the correlation of Ar-C-C_β carbon chemical shifts(ppm) of sydnone chalcones with Hammett σ , σ^+ , σ_R constants, F and R parameters. The Hammett σ_I constant was fail in correlations.

The correlation of Ar-C-CO carbon chemical shifts(ppm) of sydnone chalcones with Hammett σ , σ^+ , σ_R constants and R parameters produced satisfactory correlation coefficients. The Hammett σ_I constant and F parameters were fail in correlations.

The chemical shifts(ppm) of Ar-C-NH carbons of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ , σ^+ , σ_R constants and R parameters produced satisfactory correlation. Here, the inductive and filed components of the substituents were fail for giving satisfactory correlations.

The CS carbons chemical shifts(ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ and σ constants produced satisfactory correlation. The remaining Hammett σ_I , σ_R constants, F and R parameters were failed for producing satisfactory correlations.

The chemical shifts(ppm) of Ar-C-N⁺ carbons of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ , σ^+ , σ_I constants and R parameters produced satisfactory correlation. Here, the Hammett σ_R constant and F parameters were fail for producing satisfactory correlations.

The correlation of CO_{syd} carbons chemical shifts(ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ_I constant and F parameters produced satisfactory correlation. The remaining Hammett σ , σ^+ , σ_R constants and R parameters were failed for producing satisfactory correlations.

The chemical shifts(ppm) of Ar-C-CH₃ carbons of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ , σ^+ , σ_R constants and R parameters produced satisfactory correlation. Here, the Hammett σ_I constant and F parameters were fail for producing satisfactory correlations.

The correlation of CH₃ carbon chemical shifts(ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates with Hammett σ_I constant and F parameters produced satisfactory correlation. The remaining Hammett σ , σ^+ , σ_R constants and R parameters were failed for producing satisfactory correlations.

In single parameter correlation, some of the carbon chemical shifts of (ppm) of (*E*)-4-(*N*-(4-cinnamoylphenyl) sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates failed for production of good correlation coefficients. These are worthwhile while seeking in multi-regression analysis with σ_I and σ_R constants and Swqin-Lupton's [33]F and R parameters. The generated multi-regression equations are given in (29-50).

$$\delta\text{CO}(\text{ppm}) = 188.19(\pm 0.318) + 1.430(\pm 0.683)\sigma_I + 0.022(\pm 0.002)\sigma_R \quad (29)$$

($R = 0.962$, $n=10$, $P > 95\%$)

$$\delta\text{CO}(\text{ppm}) = 188.29(\pm 0.294) + 1.423(\pm 0.618)F + 0.480(\pm 0.527)R \quad (30)$$

($R = 0.966$, $n=10$, $P > 95\%$)

$$\delta C_\alpha(\text{ppm}) = 119.42(\pm 0.375) + 0.732(\pm 0.084)\sigma_I + 0.186(\pm 0.024)\sigma_R \quad (31)$$

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

$$\delta C_\alpha(\text{ppm}) = 119.39(\pm 0.357) + 0.872(\pm 0.074)F + 0.108(\pm 0.025)R \quad (32)$$

($R = 0.939$, $n=10$, $P > 90\%$)

$$\delta C_\beta(\text{ppm}) = 145.26(\pm 0.103) + 0.880(\pm 0.022)\sigma_I + 0.913(\pm 0.221)\sigma_R \quad (33)$$

($R = 0.991$, $n=10$, $P > 95\%$)

$$\delta C_\beta(\text{ppm}) = 145.34(\pm 0.084) + 0.791(\pm 0.147)F + 0.926(\pm 0.150)R \quad (34)$$

($R = 0.993$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-C}_\beta(\text{ppm}) = 128.03(\pm 11.358) + 1.259(\pm 0.254)\sigma_I + 0.995(\pm 0.013)\sigma_R \quad (35)$$

($R = 0.954$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-C}_\beta(\text{ppm}) = 127.99(\pm 20.358) + 1.526(\pm 0.528)F + 1.367(\pm 0.597)R \quad (36)$$

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

$$\delta\text{Ar-C-CO}(\text{ppm}) = 127.48(\pm 0.109) + 0.530(\pm 0.231)\sigma_I + 1.222(\pm 0.221)\sigma_R \quad (37)$$

($R = 0.991$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-CO}(\text{ppm}) = 127.50(\pm 0.106) + 0.518(\pm 0.022)F + 1.077(\pm 0.190)R \quad (38)$$

($R = 0.991$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-NH}(\text{ppm}) = 144.48(\pm 0.142) + 1.041(\pm 0.026)\sigma_I + 0.831(\pm 0.025)\sigma_R \quad (39)$$

($R = 0.979$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-NH}(\text{ppm}) = 144.49(\pm 0.137) + 1.366(\pm 0.394)F + 1.024(\pm 0.028)R \quad (40)$$

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

$$\delta\text{CS}(\text{ppm}) = 110.29(\pm 0.286) + 1.498(\pm 0.615)\sigma_I + 1.375(\pm 0.892)\sigma_R \quad (41)$$

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

$$\delta\text{CS}(\text{ppm}) = 110.48(\pm 0.281) + 1.329(\pm 0.089)F + 1.366(\pm 0.505)R \quad (42)$$

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

$$\delta\text{Ar-C-N}^+(\text{ppm}) = 135.82(\pm 1.108) + 1.258(\pm 0.228)\sigma_I + 0.855(\pm 0.194)\sigma_R \quad (43)$$

($R = 0.985$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-N}^+(\text{ppm}) = 135.79(\pm 1.125) + 1.245(\pm 0.262)F + 0.950(\pm 0.020)R \quad (44)$$

($R = 0.982$, $n=10$, $P > 95\%$)

$$\delta\text{CO}_{\text{syd}}(\text{ppm}) = 173.33(\pm 0.411) + 2.717(\pm 0.883)\sigma_I + 1.416(\pm 0.813)\sigma_R \quad (45)$$

($R = 0.979$, $n=10$, $P > 95\%$)

$$\delta\text{CO}_{\text{syd}}(\text{ppm}) = 173.35(\pm 0.375) + 2.751(\pm 0.789)F + 0.833(\pm 0.067)R \quad (46)$$

($R = 0.982$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-CH}_3(\text{ppm}) = 141.33(\pm 1.180) + 0.487(\pm 0.381)\sigma_I + 0.700(\pm 0.071)\sigma_R \quad (47)$$

($R = 0.964$, $n=10$, $P > 95\%$)

$$\delta\text{Ar-C-CH}_3(\text{ppm}) = 141.34(\pm 0.166) + 1.534(\pm 0.349)F + 0.662(\pm 0.158)R \quad (48)$$

($R = 0.958$, $n=10$, $P > 95\%$)

$$\delta\text{CH}_3(\text{ppm}) = 22.71(\pm 0.313) + 1.040(\pm 0.612)\sigma_I + 2.876(\pm 0.647)\sigma_R \quad (49)$$

($R = 0.987$, $n=10$, $P > 95\%$)

$$\delta\text{CH}_3(\text{ppm}) = 22.72(\pm 0.261) + 1.200(\pm 0.543)F + 2.590(\pm 0.468)R \quad (50)$$

($R = 0.990$, $n=10$, $P > 95\%$)

4. CONCLUSIONS

About ten (*E*)-4-(*N*-(4-cinnamoylphenyl)sulfamoyl)-3-(*p*-tolyl)-1,2,3-oxadiazol-3-ium-5-olates were prepared and examined their purities by literature method. The infrared and NMR spectral data were assigned and correlated with Hammett substituent constants and Swain-Lupton's constants using single and multi-regression analysis. From the results of statistical analyses, most of the single parameter correlations gave satisfactory correlation coefficients. All regression produced positive ρ values. This positive value inferred that the normal substituent effect operates

in all systems. The multi-regression analysis gave satisfactory correlation coefficients in all spectral data. In these correlations the probability factor was more than 90%. This implies that the degree of correlations was more than 90% feasible.

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