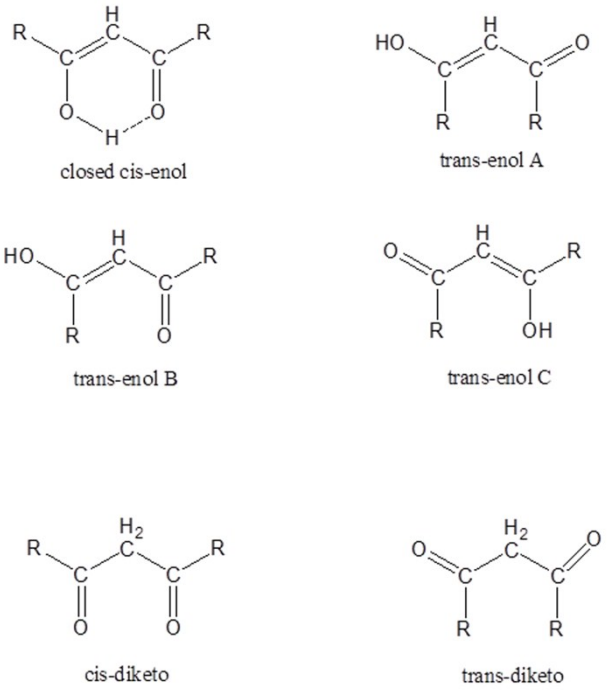
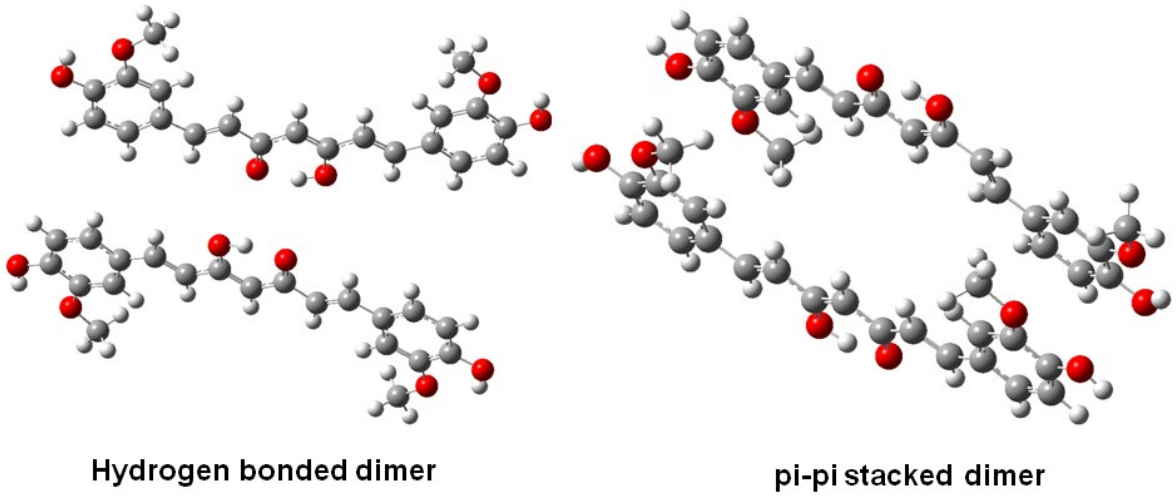
Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information



Scheme 1 Different isomeric and tautomeric forms of curcumin



Scheme 2 Two different dimeric forms of curcumin

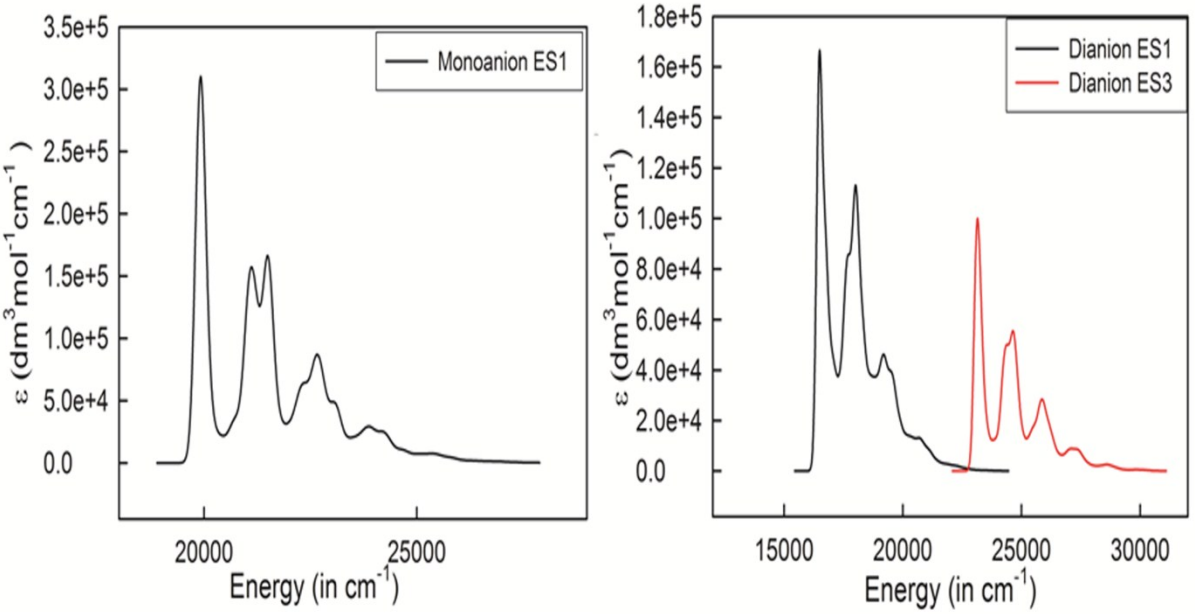


Figure S1 FC incorporated absorption spectrum of monoanionic and dianionic forms of curcumin. (The full-width at half maximum (FWHM) of 33meV are used for the convolution of the spectrum)

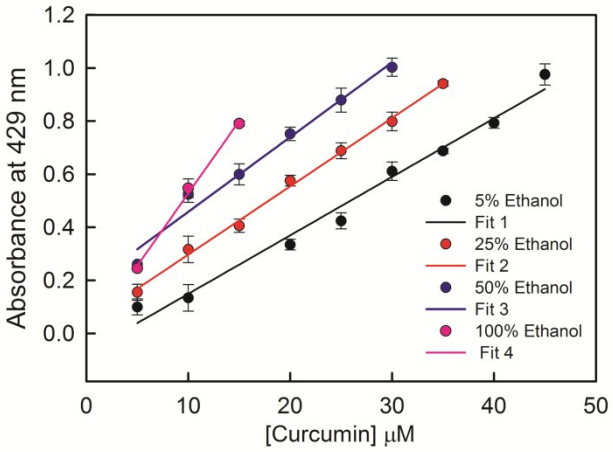


Figure S2 Calculation of molar extinction coefficient (Ɛ) of curcumin in 5%, 25%, 50% and 100 % ethanol

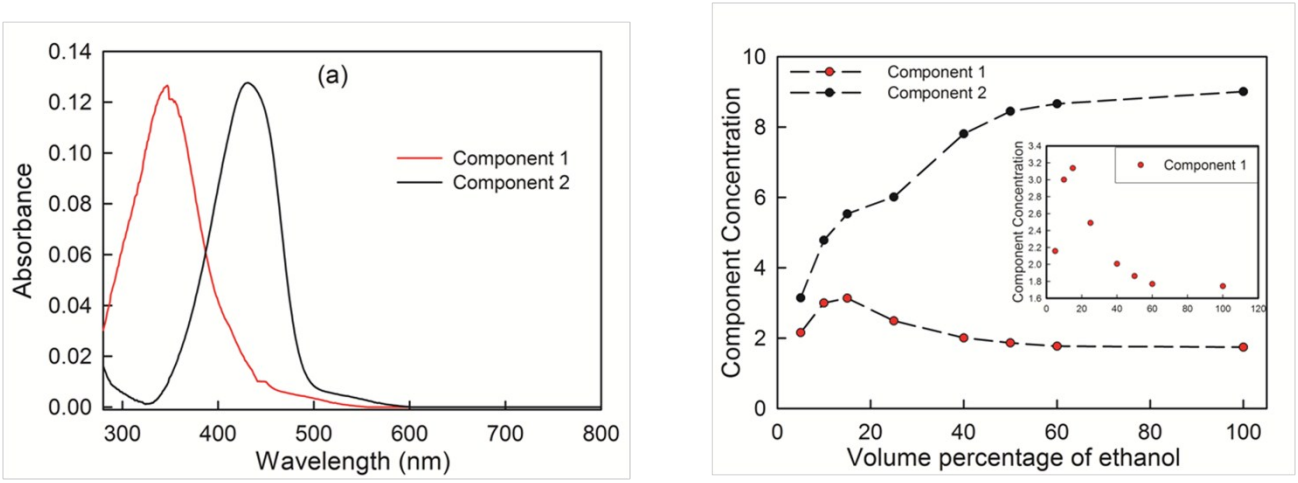


Figure S3 The pure spectra of the components and concentration distribution of the components obtained by using MCR approach

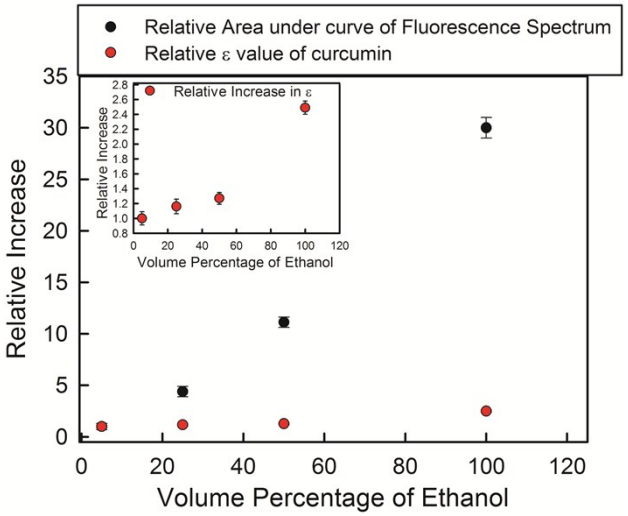


Figure S4. Relative increase in the ε_{app} value of curcumin at 429 nm (red circle) and relative increase in the area under peak at 548 nm (black circle) as a function of volume % of ethanol. There is a small change in ε_{app} value of curcumin at 429 nm as seen in Inset

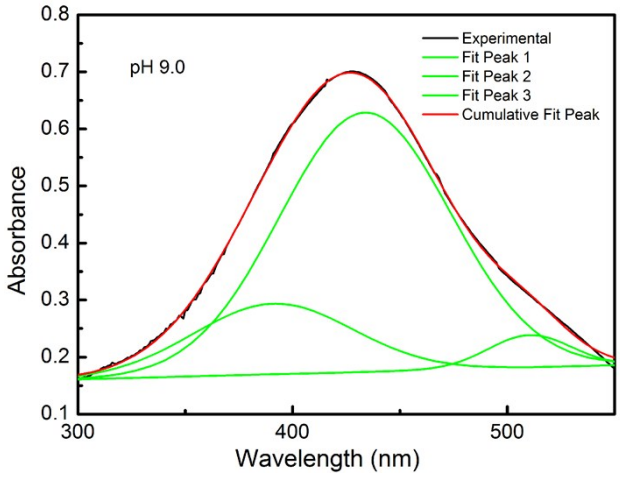


Figure S5 Resolved spectrum of curcumin (25 µM) at pH 9.0 at 25 ºC

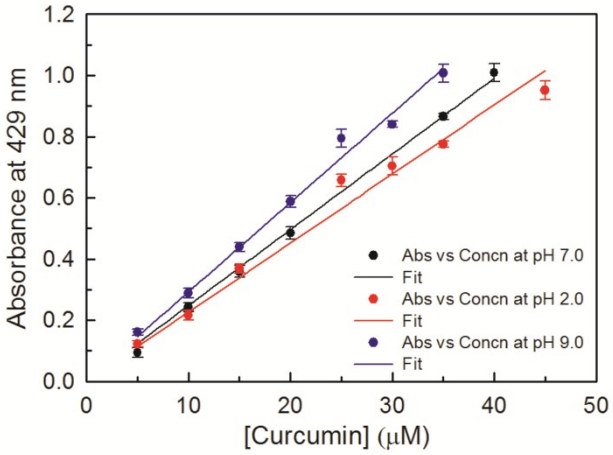


Figure S6 Calibration graph for calculation of the molar extinction coefficient (Ɛ) of curcumin pH 2.0, 7.0 and 9.0.

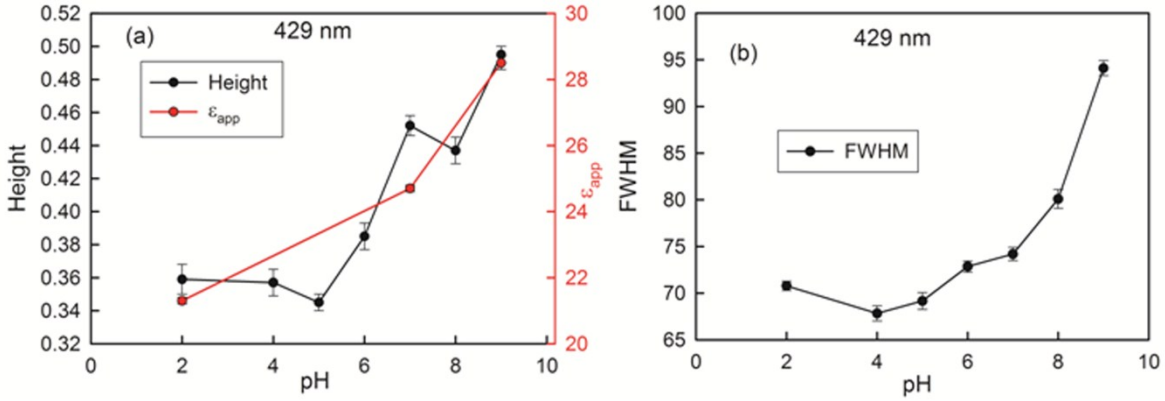


Figure S7 Change in (a) ε_{app} value of curcumin at 429 nm and absorbance (height) at 429 nm, (b) FWHM at different pH

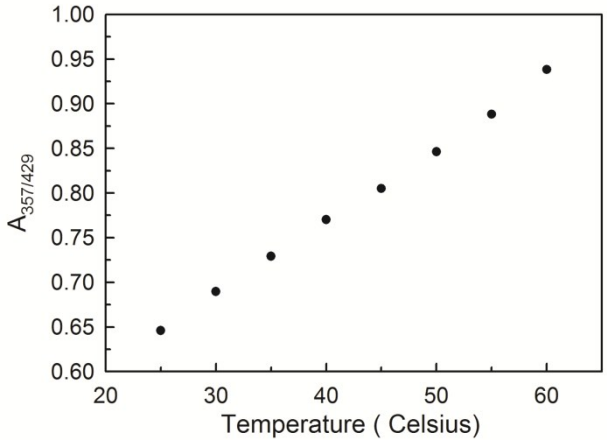


Figure S8 Ratio of A_{357}/A_{429} versus temperature (Celsius) for curcumin at pH 7.0 in 5% ethanol.

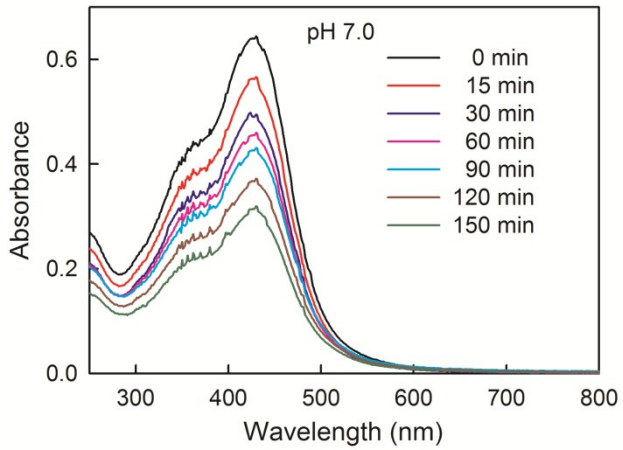


Figure S9 Absorption spectra of curcumin at pH 7.0 in 5% ethanol at different time intervals

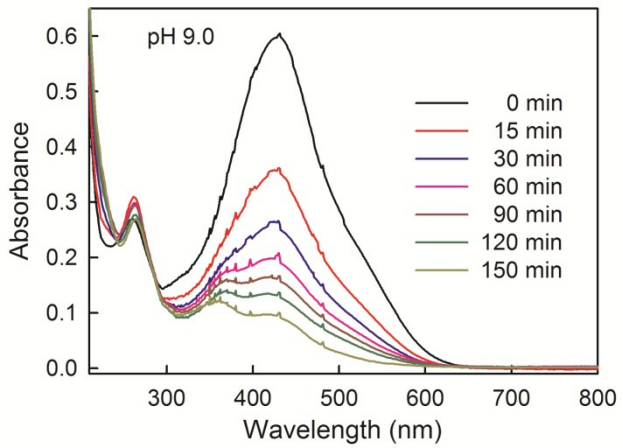


Figure S10 Absorption spectra of curcumin at pH 9.0 in 5% ethanol at different time intervals

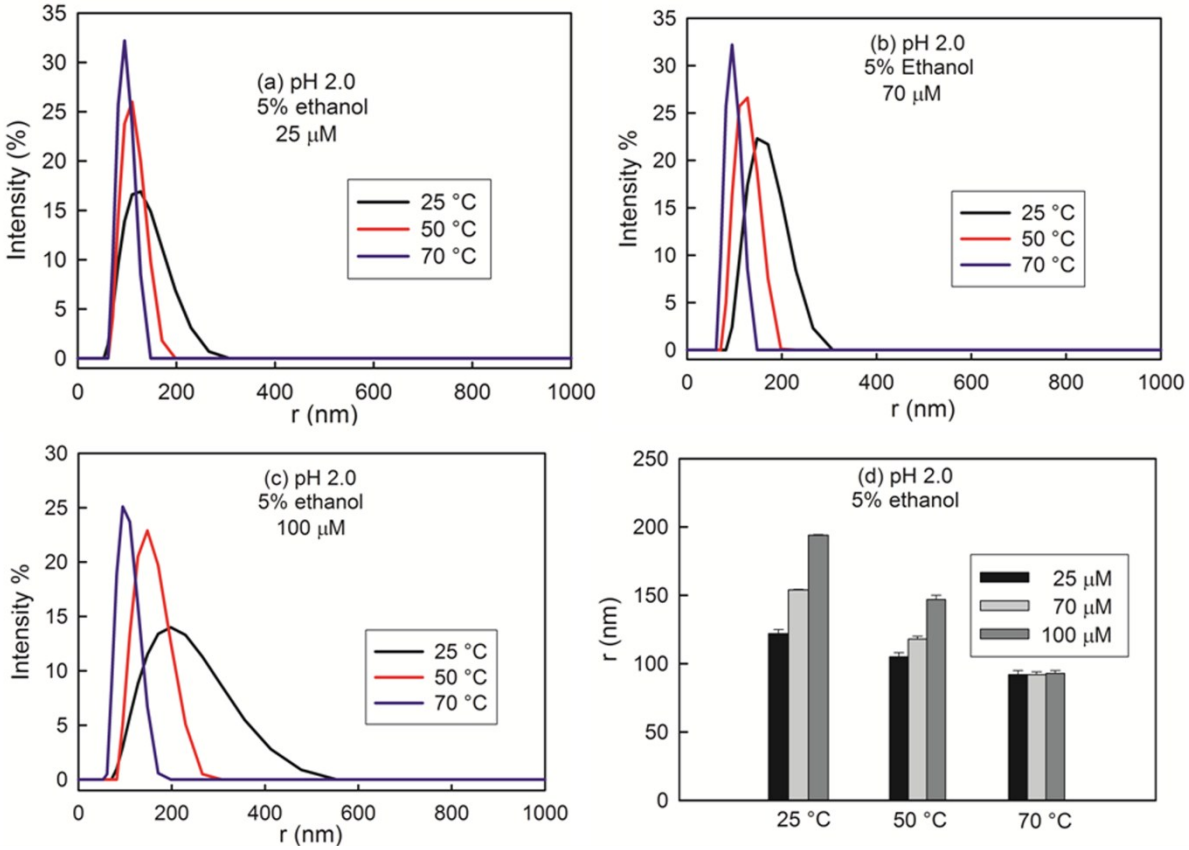


Figure S11 Particle size distribution of curcumin at different concentrations 25 μM (a), 70 μM (b), 100 μM (c) in 5% ethanolic solution. Comparison of particle size of curcumin under different conditions at pH 2.0 (d).

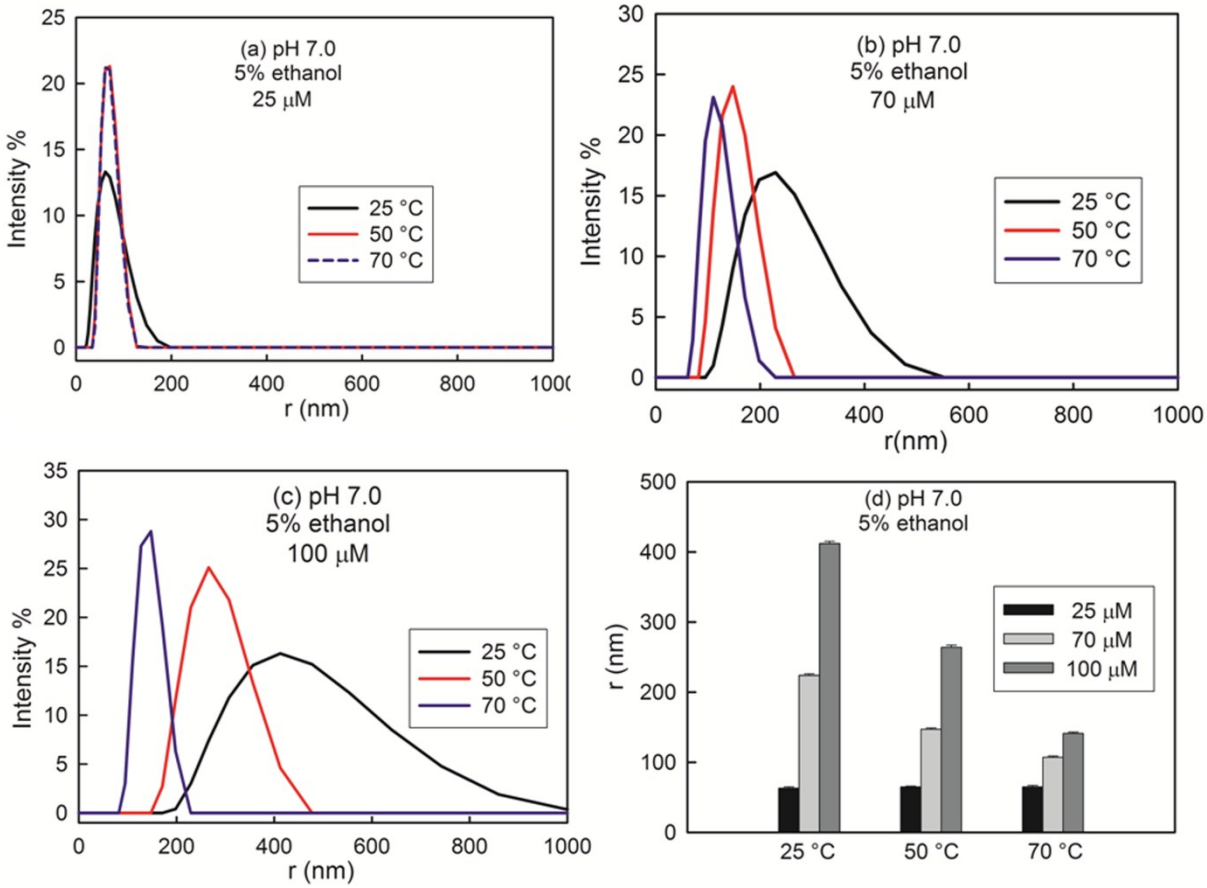


Figure S12 Particle size distribution of curcumin at different concentrations 25 μM (a), 70 μM (b), 100 μM (c) in 5% ethanolic solution. Comparison of particle size of curcumin under different conditions at pH 7.0 (d).

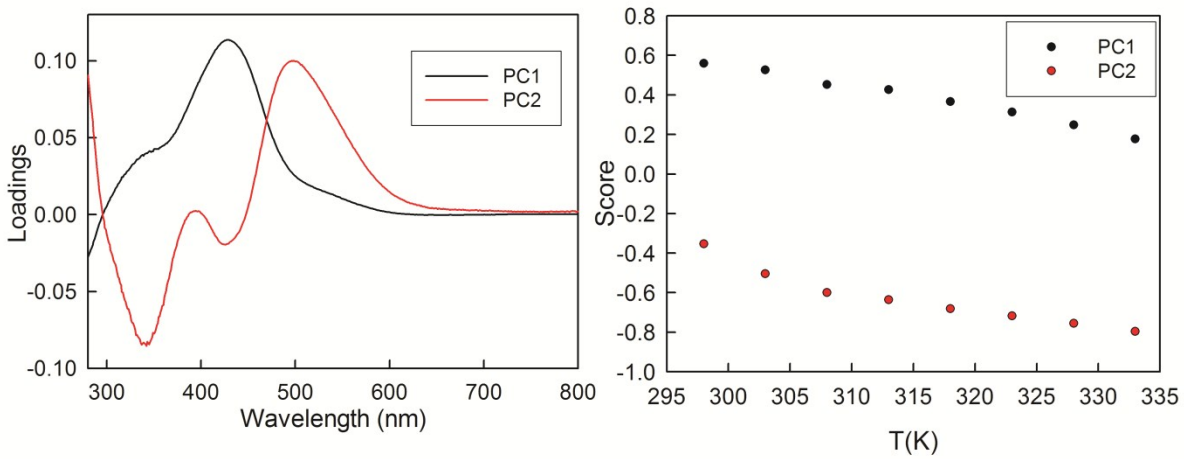


Figure S13 The loadings (left panel) and coefficient of loadings (right panel) of each principal component as determined by PCA analysis of absorption spectral variation.

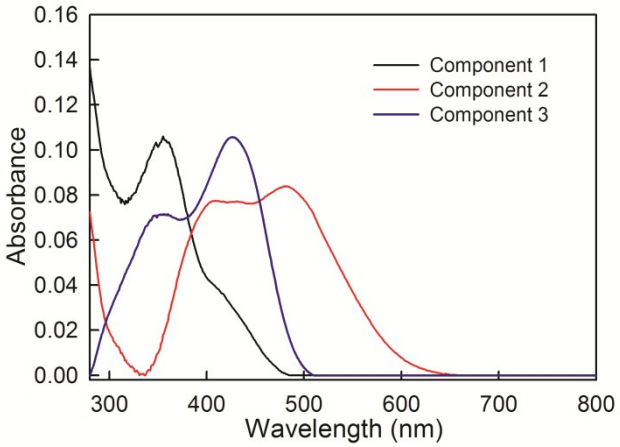


Figure S14 Number of components and pure spectra for each component extracted by employing MCR approach

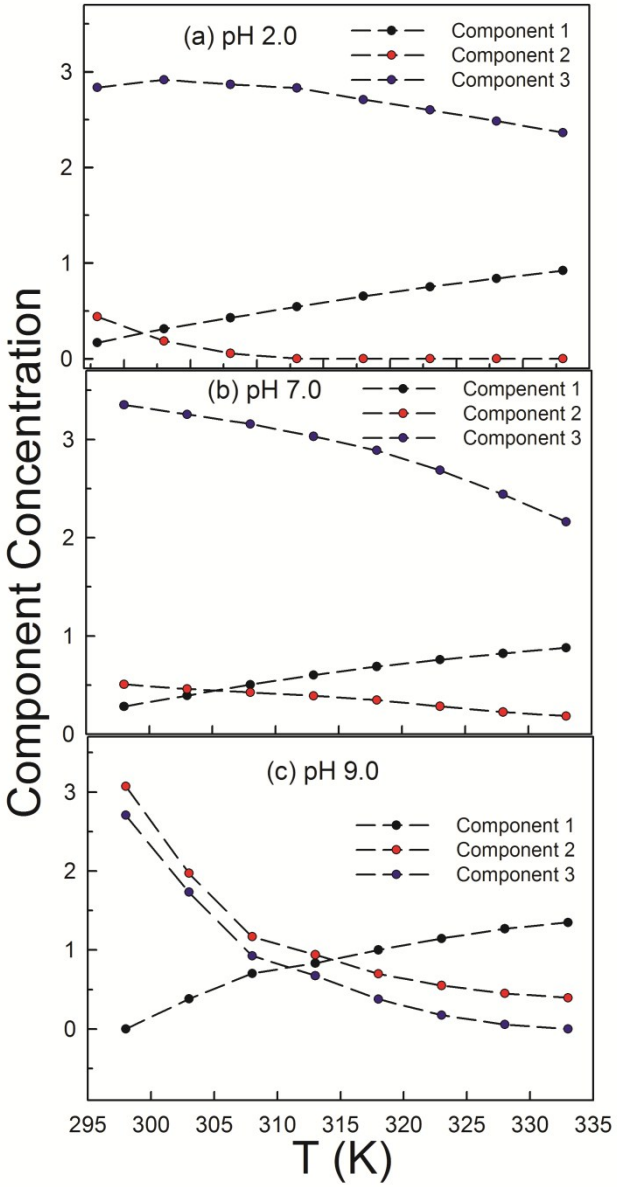


Figure S15 Concentrations of keto and enol forms estimated by MCR analysis.

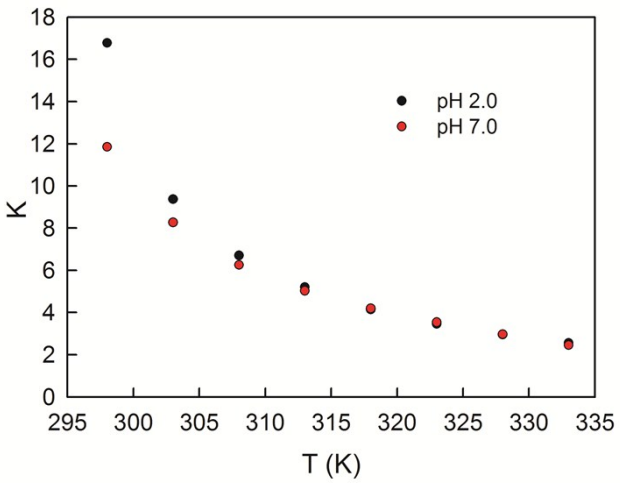


Figure S16 Variation of equilibrium constants for keto-enol tautomerization of curcumin with temperature at pH 2.0 and pH 7.0

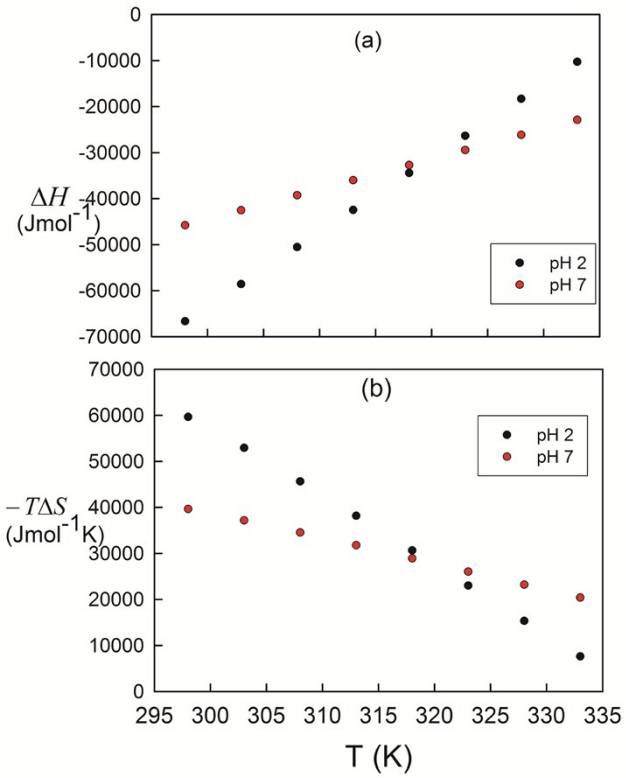


Figure S17 (a) Enthalpy and (b) Entropy compensation at pH 2.0 and pH 7.0

Table S1 Parameters (Ɛ and R^2) obtained from fitting of calibration curve of curcumin in solutions with different percentage of ethanol

	5 % ethanol	25 % ethanol	50 % ethanol	100 % ethanol
Ɛ (M^{-1} cm^{-1})	22040	25740	28160	54520
R^2	0.9792	0.9958	0.9714	0.9923

Table S2 Parameters (Ɛ and R^2) obtained from fitting of calibration curve of curcumin at different pH

	pH 2.0	pH 7.0	pH 9.0
Ɛ (M^{-1} cm^{-1})	21300	24700	28500
R^2	0.9529	0.9906	0.9842

Table S3 Thermodynamic parameters for keto-enol tautomerization equilibrium at pH 2.0

Temp (K)	K	ln K	ΔG ($Jmol^{-1}$)	ΔH_o ($Jmol^{-1}$)	ΔC_p ($Jmol^{-1}K^{-1}$)	ΔH ($Jmol^{-1}$)	ΔS ($Jmol^{-1}K^{-1}$)
298	16.77866	2.82011	-6987.026			-66623	-200.121
303	**9.37818**	**2.23839**	**-5638.822**	**-58571.71**	**1908.4**	**-58571.7**	**-174.696**
308	6.70218	1.90243	-4871.575			-50520.5	-148.211
313	5.20459	1.64954	-4292.568			-42469.2	-121.97
318	4.14852	1.42275	-3761.54			-34418	-96.4038
323	3.45736	1.24051	-3331.293			-26366.7	-71.3171
328	2.95943	1.085	-2958.786			-18315.5	-46.8191
333	2.56313	0.94123	-2605.854			-10264.2	-22.9981

Table S4 Thermodynamic parameters for keto-enol tautomerization equilibrium at pH 7.0

Temp (K)	K	ln K	ΔG ($Jmol^{-1}$)	ΔH_o ($Jmol^{-1}$)	ΔC_p ($Jmol^{-1}K^{-1}$)	ΔH ($Jmol^{-1}$)	ΔS ($Jmol^{-1}K^{-1}$)
298	11.84772	2.47214	-6124.905			-45791.6	-133.11
303	**8.26857**	**2.11246**	**-5321.587**	**-42521.13**	**654.09**	**-42521.1**	**-122.771**
308	6.25694	1.83369	-4695.552			-39250.7	-112.192
313	5.03189	1.6158	-4204.767			-35980.2	-101.519
318	4.19561	1.43404	-3791.39			-32709.8	-90.9383
323	3.54545	1.26567	-3398.858			-29439.3	-80.6207
328	2.96887	1.08818	-2967.458			-26168.9	-70.736
333	2.45549	0.89832	-2487.055			-22898.4	-61.2954