



## Adsorption affinity of tea catechins onto polymeric resins: Interpretation from molecular orbital theory

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### ABSTRACT

Adsorption of certain tea catechins such as (+) catechin (C), (–) epicatechin (EC), (+) gallic catechin (GC), (–) epigallocatechin (EGC), (+) catechin gallate (CG), (–) epicatechin gallate (ECG), (+) gallic catechin gallate (GCG), and (–) epigallocatechin gallate (EGCG) have been studied using three types of polymeric resins as adsorbents. Adsorption affinity expressed as the slope of the linear region of the isotherm for a solute is found to be different for different adsorbents, and this difference can be interpreted from the chemical nature of the sorbents. Molecular interactions on polymeric resins have been studied based on molecular orbital theory. Electronic states of adsorbent and adsorbate were calculated using the semiempirical molecular orbital (MO) method from which energy of adsorption in aqueous solution was estimated. The adsorptive interaction on the polymeric resins computed on the basis of frontier orbital theory seems to correlate well with the experimentally measured adsorption affinity and enthalpy.

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### 1. Introduction

Recently, green tea has attracted much attention both in the scientific community and in the public opinion, for its pronounced health benefits towards a variety of disorders ranging from cancer to weight loss [1]. Catechins, the principal bioactive compounds in tea are reported to have anti-tumorigenic [2,3], anti-mutagenic [4], anti-pathogenic [5] and anti-oxidative properties [6]. It is believed that much of the anticancer effects of green tea are mediated by its polyphenolic constituents due to their potent antioxidant properties and are generally considered to reflect their ability to scavenge endogenously generated oxygen radicals or those radicals formed by various xenobiotics, radiations, etc. [7].

The methodology and extraction efficiency of catechins from tea is critical in further studying the functionality of these substances. Though the classical methods of solvent extraction are available for the extraction of tea catechins, adsorption and membrane based separation methods are the most emerging and attractive from the economic viewpoint. In recent years, polymeric adsorbents have been increasingly used as an alternative to activated carbon due to their wide variations in functionality, surface area

and porosity [8–10]. Because of the high capacity, satisfactory mechanical strength and feasible regeneration under mild conditions, polymeric resins work as excellent adsorbent for removal of phenol from aqueous phase [11–13]. Huang et al. [14] have used poly(styrene-co-divinylbenzene) resin functionalized with methoxy and phenoxy groups to study the adsorption characteristics of phenols. Adsorption of phenolic compounds have also been studied by Li et al. [15] using Amberlite XAD-4 and its acetylated derivative MX-4. We have been studying membrane and adsorptive separation processes for separation and purification of some useful biomolecules using different polymeric resins and membranes as the major part of our current research program [16–23].

For a specific process application, the understanding of the sorption phenomena play crucial role in the selection of appropriate adsorbent. Adsorptive interaction and adsorption affinity are the fundamental aspects of study for assessing the feasibility of an adsorption process for practical application. Usual experimental protocol to quantify these is to determine the adsorption equilibria and enthalpy of adsorption; however, theoretical interpretation is highly essential for surface modification and/or molecular design of adsorbents with high selectivity and capacity at the same time, providing favorable adsorption isotherms. In this paper, we present both theoretical and experimental results for adsorption of certain catechins onto three commercially available structurally dissimilar polymeric sorbents in order to gain mechanistic insight into adsorption of these catechins onto polymeric resins.

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### Nomenclature

$C$	concentration of solute (mmol/l)
$C_e$	equilibrium liquid-phase concentration (mmol/l)
$C_0$	initial solute concentration (mmol/l)
$C^*$	MO coefficient
$\Delta C$	change in solute concentration (mmol/l)
$E$	stabilization energy (kJ/mol)
$E^*$	energy level of MO (kJ/mol)
$\Delta E$	perturbation energy by HOMO–LUMO interaction (kJ/mol)
$\Delta G^0$	standard free energy of adsorption (kJ/mol)
$\Delta H^0$	standard enthalpy of adsorption (kJ/mol)
$q$	amount adsorbed (mmol/g)
$R$	universal gas law constant (kJ/g/mol K)
$\Delta S^0$	standard entropy of adsorption (kJ/mol)
$T$	absolute temperature (K)
$V$	solution volume (l)
$W$	weight of adsorbent (g)
$\Delta\beta$	inter orbital interaction integral (kJ/mol)
$\Psi$	term signifying solute activity coefficient

## 2. Materials and methods

### 2.1. Materials

The catechins used in this study namely (+) catechin(C), (–) epicatechin (EC), (+) gallicocatechin (GC), (–) epigallocatechin (EGC), (+) catechin gallate (CG), (–) epicatechin gallate (ECG), (+) gallicocatechin gallate (GCG), and (–) epigallocatechin gallate (EGCG) were obtained from Sigma Chemical Co., USA. The other reagents used as buffer (potassium dihydrogen phosphate and dipotassium hydrogen phosphate) were supplied by Qualigens, India (Mumbai) and were of analytical grade. The polymeric resins Amberlite XAD-4, Dianion HP-2MG and Amberlite XAD-7 were also obtained from Sigma Chemical Co., USA. The chemical and physical properties of these resins are shown in Table 1. The adsorbents were washed with distilled water and dried overnight before use.

Equilibrium isotherms for the catechins were obtained at pH 7. The pH of solutions were measured in a pH meter and maintained at 7 by using phosphate buffer reagents of appropriate dosages. The initial concentrations of the catechins were taken between 5 and 10 mM at  $25 \pm 0.5^\circ\text{C}$  for 3–4 h, i.e. in the range of which linearity of the adsorption isotherm was obtained. Preliminary runs showed that the adsorption equilibrium adsorption was achieved after 3–4 h of contact time for all tested resins. After attainment of equilibrium, the aqueous phase was analyzed for solute concentrations by a UV–Vis spectrophotometer (Shimadzu 160A) calibrated at appropriate wavelength (280 nm) using a calibration curve of the respective catechin standards. The UV analysis was carried out in duplicate and the reproducibility was found to be  $\pm 2\%$ . For estimation of adsorption enthalpy from adsorption affinity, equilibrium experiments were conducted at two other temperatures 40 and  $55^\circ\text{C}$ . The adsorbents used were Amberlite XAD-4, XAD-7 and Dianion HP-2MG. The amounts of catechins per gram of adsorbent  $q$  (mmol/g) was calculated as  $q = V(C - C_e)/W$ , where  $C$  and  $C_e$  are the initial and equilibrium solute concentrations (mmol/l),  $V$  is the solution volume (l) and  $W$  is the weight of the adsorbent (g). All the experiments were carried out in triplicate and the reproducibility was found to be  $\pm 2\%$ .

The numerical values of the adsorption affinity ( $q/C_e$ ) can be determined by two techniques; (1) individual values of  $q/C_e$  can be averaged and (2) the slope of the best-fit line for the isotherms can be evaluated. For adsorption equilibrium studies low concen-

trations of catechins were used to limit the adsorption to the linear region of the isotherm where all of the isotherms could be extrapolated to the origin. The adsorption affinities ( $q/C_e$ ) were determined from the slopes of individual isotherms in the linear region and the values are identical to the averaged values of individual adsorption affinities.

### 2.2. Adsorptive interaction in aqueous solutions

#### 2.2.1. Molecular orbital (MO) calculation

Molecular orbital provides information on the basis of electronic states of adsorbents in an adsorption system, which will exploit to sorbent–solute interactions. In order to calculate electronic states of adsorbents by MO (molecular orbital) method, it is necessary to provide a structural (molecular) model of the adsorbents as discussed by previous workers and we have extended successfully the model for calculation of  $\beta$ -lactum antibiotics and some other biomolecules on polymeric resins [10]. Recently, the MO theory has been exploited to correlate Freundlich isotherm parameter for adsorption of phenols, 4-chlorophenols, and 3-nitrophenols on Amberlite XAD-2000 [24]. Mardis et al. [25] have calculated standard free energy of binding using quantum mechanical calculations to elucidate the mechanism of selectivity of oxygenated aromatic compounds onto acrylic ester sorbent XAD-7. Like our earlier work [10,16], we use a styrene-divinylbenzene (SDVB) polymer as the cluster model of synthetic adsorbent XAD-4 as shown in Fig. 1(a). Fig. 1(b) gives the cluster model of synthetic adsorbent XAD-7, which is an aliphatic carboxylic acid polymer. We use a methacrylate polymer as the cluster of synthetic adsorbent HP-2MG as shown in Fig. 1(c). Tamon et al. [26] have used cluster models to study the adsorptive interaction of organic compounds on activated carbon and synthetic adsorbents. The cluster size is very important in the MO calculation. If the cluster size is small, the size seriously influences the electronic state of adsorbent surface. So, we have calculated the electronic state of the cluster models adopting the minimum cluster size to get the more appreciable influence on the energy level.

The electronic state of adsorbents and adsorbates can be determined by semiempirical molecular orbital calculations. Though several semiempirical MO methods such as Austin model (AM1), complete neglect of differential overlap (CNDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of differential overlap (MNDO), parameterized model number 3 (PM3), and parameterized model number 5 (PM5) can be used for calculation of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, the basis of which may be understood from the solute–solvent model (Fig. 2). However, in our case we have used PM5 as it gives satisfactory results because all the parameters for most of the atoms are available in PM5. All these methods are semiempirical and used for the quantum calculation of molecular electronic structure in computational chemistry and based on the neglect of differential diatomic overlap integral approximation. The interaction energy between adsorbate and adsorbent is calculated on the basis of the frontier orbital theory (FOT) proposed by Fukui et al. [27]. According to FOT, two body interactions such as adsorbent–adsorbate, adsorbent–solvent, are regarded as the mixing of HOMO and LUMO. The HOMO energy is a measure of how hard it is to remove an electron from a neutral molecule and the LUMO energy is a measure of how hard it is to add an electron to the neutral molecule. Fig. 2 shows the concept of MO mixing. In this figure, molecule A is electron donating, and molecule B is electron attracting. Considering the charge transfer from atom  $r$  of molecule A to  $s$  of molecule B the energy level of HOMO of molecule A changes to the more stable level by orbital mixing. On the other hand, the energy level of LUMO of molecule B attains a more unstable level. The energy dif-

**Table 1**  
Chemical and physical properties of resins reported by manufacturers.

Trade Name	Structure	Surface area (m <sup>2</sup> /g)	Pore radius (Å)	Wet mesh size	Particle size (mm)	Density (g/ml)
Amberlite XAD-7	Acrylic	450	45	20–60	0.25–0.84	1.24
Amberlite XAD-4	SDVB	725	20	20–60	0.25–0.84	1.02
Dianion HP-2MG	Acrylic	500	85	20–60	0.3–0.6	1.09

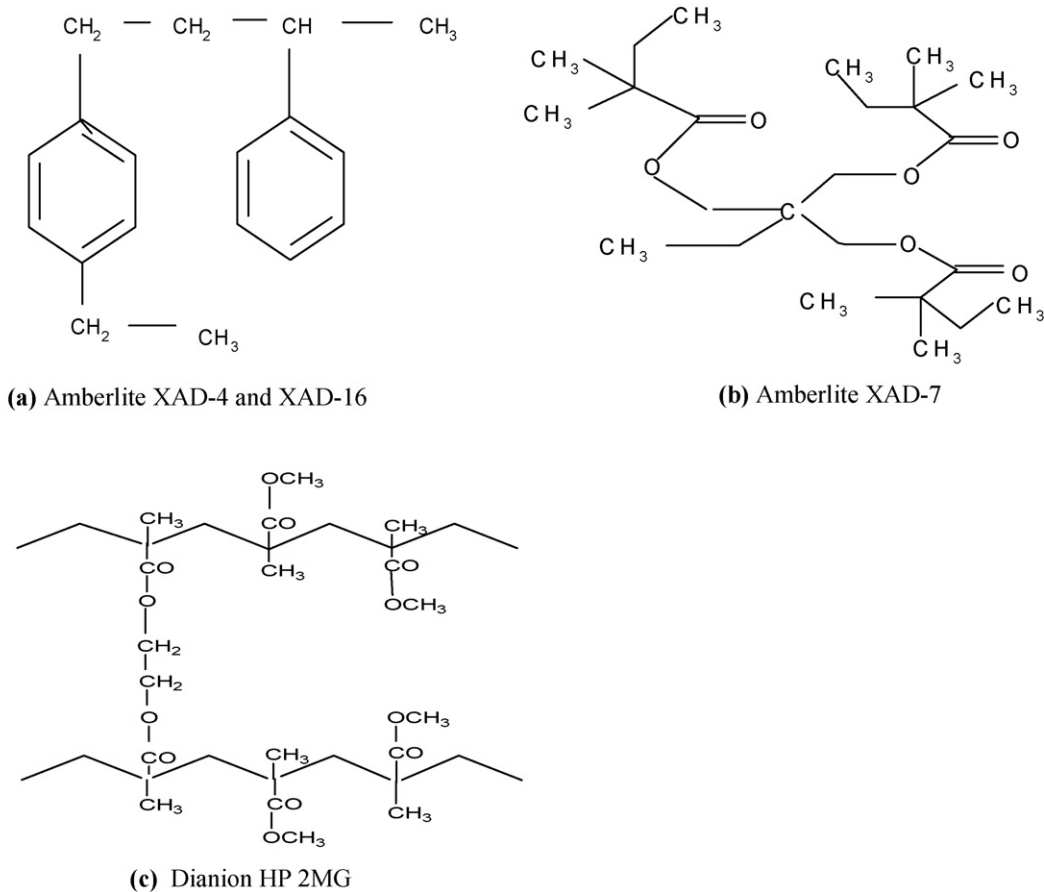


Fig. 1. Cluster model of adsorbent surface.

ference  $\Delta E$  shown in Fig. 2 is called perturbation energy. The second order perturbation expression for the energy that accompanies the interaction can be derived, and the perturbation energy  $\Delta E$  caused by the HOMO–LUMO interaction as calculated by Tamon et al. [26] which is given by Eq. (1)

$$\Delta E = \frac{2(C_r^* C_s^* \Delta\beta)^2}{|E_a^* - E_b^*|} \quad (1)$$

where  $E_a^*$  and  $C_r^*$  are the HOMO energy and orbital coefficient of the atom “r” of electron attracting molecule “a”, respectively. Respectively,  $E_b^*$  and  $C_s^*$  are the LUMO energy and the orbital coefficient of atom “s” of electron donating molecule “b”. For MO calculation of adsorbent and adsorbate molecules we used MOPAC available in Quantum CAChe software. The optimized geometry of the catechins and cluster model of adsorbents can be found by minimizing their total energies with respect to the corresponding geometric variables i.e. bond length, bond angles and dihedral angles. Then the optimized structures were run in the PM5 Hamiltonian for semiempirical calculations. The output of the computer aided programme gives the HOMO–LUMO energies and their respective orbital coefficients of the required atoms. The square of the coefficient indicates the existence probability of an electron, and the 1S orbital for H atom, 2P<sub>x</sub>, 2P<sub>y</sub> and 2P<sub>z</sub> orbitals for

C, O, N and S were taken into account to estimate  $\Delta E$ .  $\Delta\beta$  is the inter orbital interaction integral between the interacting orbitals of atoms, which is proportional to the overlap integral. Once the frontier orbital model is assumed, the choice of distance separating the interacting orbitals is important as the values of  $\Delta\beta$  depend on the distance. We have chosen a distance of 0.242 nm because only at a distance of 0.25 nm, the positive lobe of one orbital starts overlapping the negative of the other and vice versa [28]. The following values of  $\Delta\beta$  at 0.242 nm are used to calculate  $\Delta E$ , 3.00 eV for C–C, 2.49 eV for C–O and 2.00 eV for O–O [26]. Eq. (1) indicates that  $\Delta E$

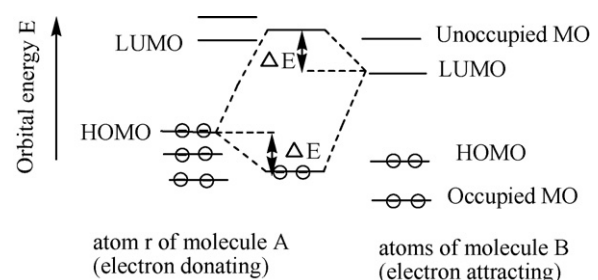


Fig. 2. Concept of molecular orbital mixing [26].

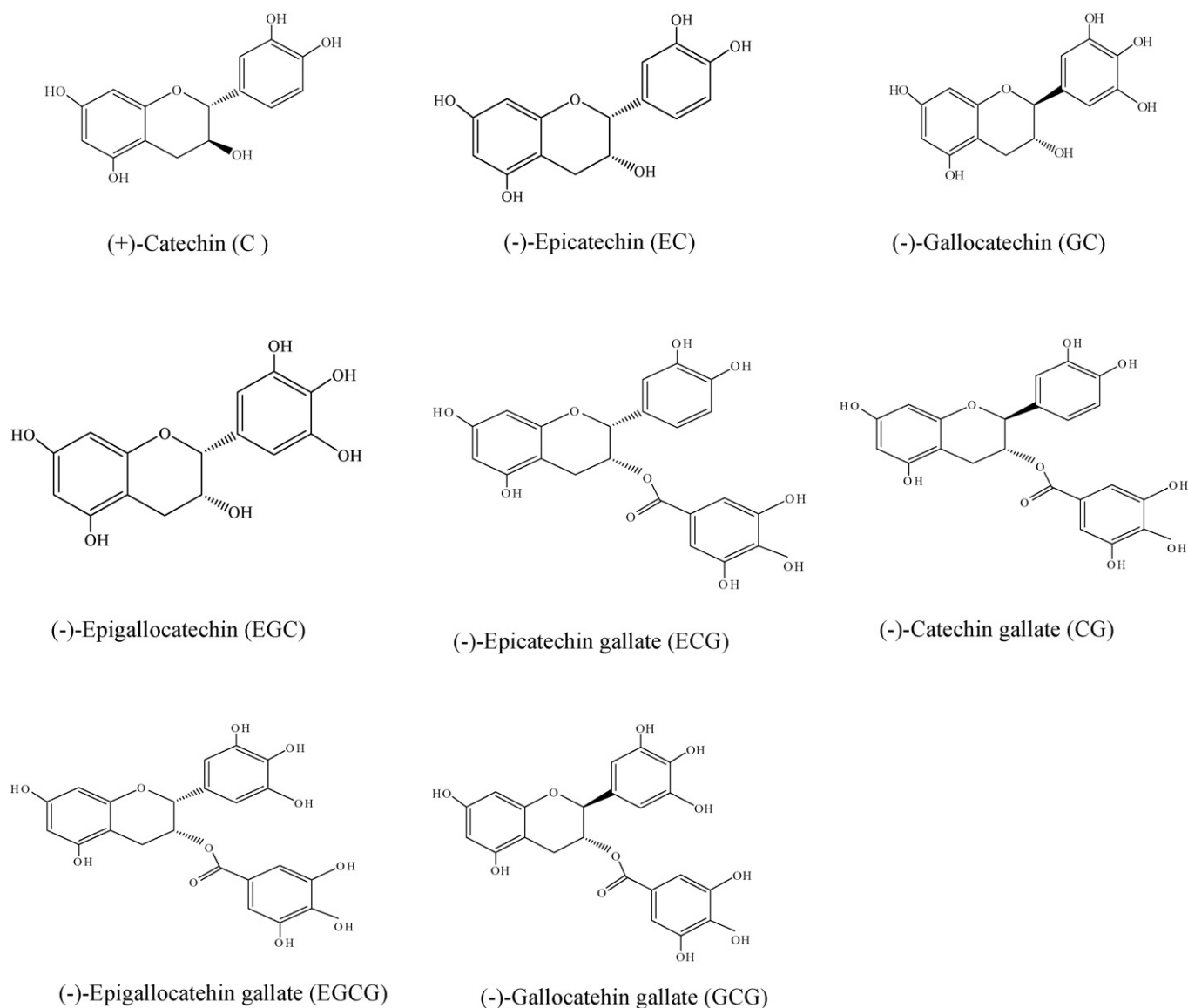


Fig. 3. Structures of eight green tea catechins.

is large when  $|E_a^* - E_b^*|$  is small. Hence,  $|E_a^* - E_b^*|$  is an index of the strength of adsorptive interaction on the adsorbent surface.

### 3. Results and discussion

#### 3.1. Adsorption equilibrium

The adsorption equilibria were interpreted from Langmuir, Freundlich and Redlich–Peterson isotherms. Table 2 shows the values of the isotherm parameters estimated by non-linear regression analysis. It appears that out of three isotherm model studied both Langmuir and Redlich–Peterson model provides identical fit of experimental data at almost for all the adsorbents studied. However, representation of experimental data for Freundlich isotherm model appears to be relatively inferior which is contradictory to the observations made by Silva et al. [29] for adsorption of polyphenols on macroporous resins and Ye et al. [30] for adsorption of tea catechins onto lignocellulose.

Experimentally obtained adsorption equilibria which were characterized in terms of the affinities, can be related to adsorption enthalpy and interaction energy [16]. The adsorption affinity

( $q/C_e$ ) is defined as the equilibrium ratio of the solid-phase concentration (mmol/g sorbent) to the liquid-phase solute concentration (mmol/l). The adsorption affinities for each of the catechins are reported in Table 3. These values alone are considered for estimation of adsorption enthalpies where have been correlated with adsorptive interaction energies. The structures of the catechins are shown in Fig. 3 as these were utilized in executing molecular orbital calculations.

#### 3.2. Correlation of adsorptive affinity with interaction energy

The adsorption affinity of XAD-7 is higher than that exhibited by Dianion HP-2MG and XAD-4 for all the catechins studied in this work as can be seen from Table 3. Usually adsorption is affected by external physicochemical parameters such as pH, temperature, competing compounds present in solution, and on the chemical structure and other characteristic properties of the adsorbent such as particle size, porosity, polarity, specific surface area, and pore volume distribution. Surface area and pore radius keeps a linear relation with adsorption capacity with pore radius  $\leq 90 \text{ \AA}$  [29]. However, these parameters have not been explicitly consid-

**Table 2**  
Parameter values for the adsorption isotherms of (+)-catechin at 25 °C.

Adsorbent	Langmuir $q = KX_m/(1 + KC_e)$			Freundlich $q = K_F C_e^n$			Redlich–Peterson $q = KC_e/(1 + a_R C_e^b)$			
	K	$X_m$	$R^2$	$K_F$	n	$R^2$	K	$a_R$	b	$R^2$
Amberlite XAD-7	1.4381	1.9495	0.9957	1.0507	0.5314	0.9707	1.8224	1.7345	0.4685	0.9946
Amberlite XAD-4	0.0369	1.4457	0.9862	0.3914	0.5568	0.9850	1.0474	1.6625	0.6197	0.9854
Dianion HP	0.9394	2.0552	0.9958	0.9044	0.5570	0.9793	1.2713	1.4055	0.4429	0.9958

**Table 3**  
Adsorption affinity for catechins onto different adsorbents at pH 7.

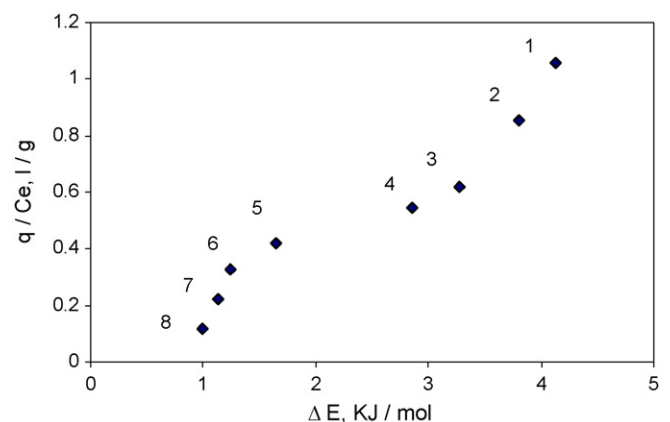
Adsorbate	Adsorbent	Adsorption affinity $q/C_e$ (l/g)	Adsorption enthalpy $\Delta H$ (kJ/mol)
ECG	Amberlite XAD-7	1.0568	9.25
	Amberlite XAD-4	0.5962	6.53
	Dianion HP-2MG	0.8212	7.01
EC	Amberlite XAD-7	0.8564	8.29
	Amberlite XAD-4	0.4959	5.25
	Dianion HP-2MG	0.7209	6.04
C	Amberlite XAD-7	0.6166	7.12
	Amberlite XAD-4	0.3606	4.22
	Dianion HP-2MG	0.4681	5.12
GCG	Amberlite XAD-7	0.5465	6.58
	Amberlite XAD-4	0.2802	4.12
	Dianion HP-2MG	0.3310	4.65
GC	Amberlite XAD-7	0.4215	5.69
	Amberlite XAD-4	0.1124	3.56
	Dianion HP-2MG	0.2091	3.95
CG	Amberlite XAD-7	0.3265	4.95
	Amberlite XAD-4	0.0959	2.98
	Dianion HP-2MG	0.1909	3.55
EGCG	Amberlite XAD-7	0.2256	4.56
	Amberlite XAD-4	0.0713	2.19
	Dianion HP-2MG	0.1133	2.71
EGC	Amberlite XAD-7	0.1145	3.21
	Amberlite XAD-4	0.0564	2.11
	Dianion HP-2MG	0.0989	2.56

ered for the interpretation of the correlation between adsorption affinity and interaction energy. For a given sorbent, adsorption is generally believed to result from two types of driving forces. Specific driving forces result from solute–sorbent interactions and depend on the sorbent surface chemistry. Non-specific driving forces are independent (or less dependent) of the surface and result primarily from solute–solvent interactions, which tend to drive organics from water (e.g. hydrophobic interactions). The adsorption of polyphenols by resins containing amide groups is driven by hydrophobic interaction and multiple hydrogen bonding [31,32]. Phenol molecules adsorb effectively from aqueous solutions onto the acrylic ester polymer through van der Waals interaction, while from their hexane solution can be achieved onto Amberlite XAD-7 primarily through the intermolecular hydrogen bond formed between the phenolic hydroxyl group and the carbonyl group on the polymeric matrix [33,34]. Such specific interaction may play a positive role in phenol adsorption from aqueous solution [35], however, adsorption driven by hydrogen bonding alone in aqueous solution is very weak because of the strong hydrogen bonding characteristics of water [25,32].

In addition, the competition between different catechins for the adsorption sites, may vary and with some catechins being preferentially selected than others. Furthermore, solubility and adsorption are inversely related. The solubility is affected by the solvophobicity of a compound, and the greater its solvophobicity with respect to a given solvent, the greater its tendency to be adsorbed from that solvent at interfaces with other phases [36]. However, in our study chemical nature of the adsorbents used plays more important role than their characteristic physical properties for adsorption of catechins. Amberlite XAD-7, which gives the highest affinity for all the adsorbate molecules is a non-ionic aliphatic acrylic polymer whereas XAD-4 is composed of styrene-divinylbenzene, a

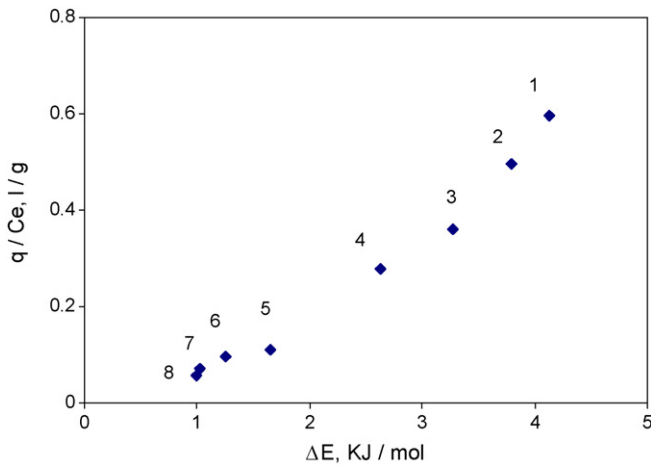
hydrophobic polyaromatic polymer, making them more efficient for adsorption of compounds of higher hydrophobicity. Dianion HP-2MG, which is also a non-ionic aliphatic acrylic polymer, shows intermediate affinity for the adsorbates. So the high affinity of all the adsorbate molecules for XAD-7 may be due to the hydrophilic nature of the polyphenols. Therefore, polarity matching between XAD-7 among the resins used here and polar adsorbate may partially account for the increase in adsorption capacities. Silva et al. [29] have also found similar results for adsorption of polyphenols on macroporous resins.

The adsorptive interaction energy  $\Delta E$ , calculated by using Eq. (1) is correlated with adsorption affinity of eight tea catechins. The results shown in Figs. 4–6 indicate a unique relationship between

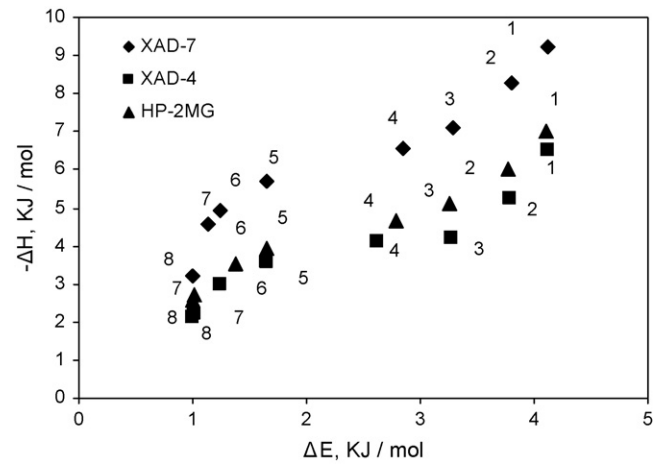


**Fig. 4.** Plot of affinity versus interaction energy on XAD-7. ECG (1), EC (2), C (3), GCG (4), GC (5), CG (6), EGCG (7), EGC (8).

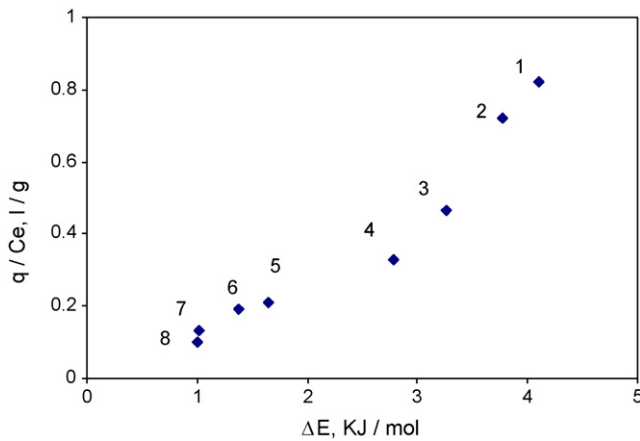




**Fig. 5.** Plot of affinity versus interaction energy on XAD-4. ECG (1), EC (2), C (3), GCG (4), GC (5), CG (6), EGCG (7), EGC (8).



**Fig. 7.** Plot of adsorption enthalpy vs. interaction energy on different polymeric resins. ECG (1), EC (2), C (3), GCG (4), GC (5), CG (6), EGCG (7), EGC (8).



**Fig. 6.** Plot of affinity versus interaction energy on HP-2MG. ECG (1), EC (2), C (3), GCG (4), GC (5), CG (6), EGCG (7), EGC (8).

adsorptive affinity and adsorptive interaction for all the catechins tested. It can also be inferred from these figures that the adsorbent which shows highest affinity, also shows the highest interaction energy, i.e.  $\Delta E$ . Similarly, the adsorbent exhibiting the lowest affinity also shows the lowest interaction energy implying that the polarity of the sorbent affects the adsorption equilibrium [10,18]. This indicates much stronger specific interactions between the polar carbonyl groups on the XAD-7 resin with the water soluble, hydrophilic tea catechin sorbates. Andrzej et al. [37] have also reported stronger interactions for hydrophilic, water soluble solutes on sorbents having polar groups.

### 3.3. Correlation adsorption enthalpy with interaction energy

Van't Hoff method utilizing the temperature dependence of the adsorption affinity,  $q/C_e$  ( $C_e$  being the equilibrium solute concentration) has been adopted to estimate the adsorption enthalpy. The first thermodynamic relationship being:

$$\Delta G^0 = RT \ln K = -RT \ln \left\{ \Psi \left( \frac{q}{C_e} \right) \right\} \quad (2)$$

where  $\Delta G^0$  is the standard free energy of adsorption,  $R$  is the universal gas constant,  $T$  is the temperature in Kelvin,  $K$  is the equilibrium constant for the adsorption process and  $\Psi$  is a proportionality constant which includes terms for the activity coefficients of the solute in the two phases and the activity of the unbound adsorption sites.

By confining our studies to low solute concentration, adsorption was limited to the linear region of the isotherm, and therefore we believe that the equilibrium constant can be directly related to the adsorption affinity [38]. Since we confined our studies to a narrow range of solute concentrations (in both the solid and liquid phases), it is possible that  $\Psi$  will be constant over the condition applied.

The second thermodynamic relationship used in the Van't Hoff method is:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad (3)$$

where  $\Delta H^0$  and  $\Delta S^0$  are the standard enthalpy and entropy changes of adsorption, respectively. Combining Eqs. (2) and (3), we have:

$$\ln \left( \frac{q}{C_e} \right) = \frac{-\Delta H^0}{RT} + \left[ \frac{\Delta S^0}{R - \ln \Psi} \right] \quad (4)$$

If  $\Delta H^0$ ,  $\Delta S^0$  and  $\Psi$  remain constant over the temperature range studied, a plot of  $\ln(q/C_e)$  versus  $1/T$  yields a straight line with a slope of  $-\Delta H^0/R$ , from which  $\Delta H^0$  can be calculated. Van't Hoff plots were used by Ye et al. [30] to calculate enthalpy and entropy changes of catechin adsorption onto lignocellulose. The temperature effect of the adsorption equilibrium was evaluated by measuring the adsorption at three different temperatures, i.e. 25, 40 and 55 °C and at a constant pH of 7. The enthalpy of adsorption was estimated from the Van't Hoff plots of  $\ln(q/C_e)$  versus  $1/T$  given by Eq. (4) and the parameters were estimated by linear regression of the data within the range of temperature studied in this work. The experimentally obtained adsorption enthalpy ( $\Delta H^0$ ) values are plotted against adsorptive interaction energies ( $\Delta E$ ) as shown in Fig. 7, which shows a reasonable linear relationship an observation a keen to that obtained for the adsorption of  $\beta$ -lactum antibiotics on polymeric resins [10,18]. The differences in the adsorption enthalpies of the solutes onto different polymeric adsorbents (as shown in Table 3) can be exploited for selective adsorption in practical situations. A strong correlation between the adsorption affinity and the adsorption enthalpy was also observed for the adsorption of *N*-methylaniline, alcohols, and phenols on polycarboxylic ester sorbent [38]. Since the enthalpy is a measure of the strength of the solute–sorbent binding interaction, the correlation illustrated in Fig. 7 demonstrate that the polarity of the sorbent is significantly responsible for binding of catechin molecules and the process may be considered to be of enthalpic type. This implies that the enthalpies of adsorption are in conformity with adsorptive interaction energy.

#### 4. Conclusion

Adsorption interaction energies between eight major tea catechins and three different adsorbents such as Amberlite XAD-7, Dianion HP-2MG and XAD-4 were calculated using molecular orbital theory. The computational and experimental studies described here provide further insight into the mechanisms by which catechins bind to the surface of the acrylic ester sorbents and SDVB sorbents. These theoretical results show good correlations with experimental results on adsorption affinity and enthalpy. This gives evidence that polarity of the solute affects the adsorptive interaction of catechins in aqueous solution on polymeric resins. The results have stimulated the development of alternative sorbents which confer high selectivity and capacity for liquid-phase adsorption of catechins by limiting adsorption to specific interactions [10,31,38]. The development of such sorbents has been greatly facilitated by advances in polymer synthesis methods, which has made it possible to produce polymeric sorbents of well-characterized and uniform chemical surfaces. Accordingly, these results are expected to provide implication for sorbent surface modification and better design of adsorbents with high selectivity and capacity for liquid-phase adsorption of catechins.

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