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Chapter

QSPR Prediction of Chromatographic Retention Times of Tea Compounds by Bioplastic Evolution

Francisco Torrens and Gloria Castellano

Abstract

Structure-property relationships model the ultrahigh-performance liquid chromatographic retention times of tea compounds. *Bioplastic evolution* presents a viewpoint in evolutionary science. It conjugates the result of acquired characters and associations rising between three rules: *evolutionary indeterminacy*, *morphological determination*, and *natural selection*. It is used to propose the co-ordination index, which is utilized to describe the retentions of tea constituents. In molecules, three properties allow computing the co-ordination descriptor: the molar formation enthalpy, molecular weight, and surface area. The result of dissimilar kinds of characteristics is examined: thermodynamic, *steric*, geometric, lipophilic, etc. The features are molar formation enthalpy, molecular weight, hydrophobic solvent-accessible surface area, decimal logarithm of the 1-octanol/water partition coefficient, etc. in linear and quadratic associations. The formation enthalpy, molecular weight, hydrophobic surface, partition, etc. differentiate the molecular structures of tea components. Feeble quadratic associations result between partition, hydrophobic surface and retention. The morphological and co-ordination descriptors complete the associations.

Keywords: biological plastic evolution, morphological index, co-ordination index, formation enthalpy, lipophilicity, solvent-accessible surface, solvation parameter model, metabolomics, metabolic profiling, catechin derivative, polyphenol, green tea, black tea

1. Introduction

Fast separation of complex samples, via high-resolution (HR) chromatography and mass spectrometry (MS), requires meeting the simultaneous need of high sample throughput and high-quality (HQ) data in metabolomics. Hyphenation of ultrahigh-performance liquid chromatography (LC) (UHPLC) and maXis ultra-HR time-of-flight (UHR-TOF)-MS delivers speed without compromising performance factors, e.g., sensitivity, mass accuracy, and resolution. Black tea (BT) and green tea (GT), *Camellia sinensis* L. (Theaceae), account for 95% of the world tea consumption [1]. The health benefits of BT and GT are hypothesized. Understanding the potential health-promoting effects and improvement in quality/taste is interesting. In BT production, GT leaf catechin (GTC) (glycosylated) flavan-3-ol flavonoids are

enzymatically oxidized (*fermented*) to yield a complex mixture of products, e.g., theaflavins (TFs) and thearubigins (TRs). Despite the importance of tea beverages, most chemical constituents were not confirmed because of mixture complexity. Antioxidant activity (AOA) of standard (gallated) GTCs decays as follows: (−)-epigallocatechin (EGC) 3-*O*-gallate (EGCg) > (+)-gallocatechin (GC) 3-*O*-gallate (GCg) > (−)-epicatechin (EC) 3-*O*-gallate (ECg) > EGC > GC > EC > (+)-catechin (C) [2]. The contents of *cis*-GTCs are the key factors affecting GT AOA. GT, *oolong* (blue) tea (OT), and BT are unoxidized, semi-oxidized, and oxidized, respectively, during production. Darjeeling tea is sold as *BT* but it belongs to OTs. The oxidation grade of tealeaves rises GT < OT < BT. GTCs are excellent electron donors (EDs) and effective traps (*scavengers*) of physiologically relevant *in vitro* reactive oxygen species (ROSs).

Data generated from BT, GT, and Darjeeling tea extracts were analyzed via UHR-TOF-MS, with electrospray ionization (ESI) in negative ion (NI) mode [3]. Mass data and isotopic pattern information in MS/MS-MS spectra enable the sum formula generation. Combining the formulae with database (DB) queries facilitates the identification of unknown compounds. Some tea polyphenolic compounds and metabolites penetrate the blood-brain barrier (BBB) into brain regions, which mediates cognition. In rats, trihydroxybenzoic acid glycoside theogallin or its metabolite cyclitol, cyclic polyol, *cyclo*hexanecarboxylic quinic acid moved via BBB and presented cognition-enhancing activities [4]. The effects of flavonoids on the central nervous system (CNS) were reviewed [5]. Flavan derivative, flavan-3-ol EC, is able to cross BBB more efficiently than stilbenoid resveratrol, which is more hydrophilic. Polyphenols entering the brain were revised [6]. The potential role of GTCs in the prevention of the metabolic syndrome was re-examined [7]. The clinical evidence of GT effects was discussed [8]. The GTCs and caffeine (Caff) and their synergism in body weight regulation were reviewed [9]. The antiobesity effects of GTCs were revised [10]. The chemistry of low-molecular-weight BT polyphenols [11], and secondary ones produced during tea processing [12], was re-examined. The content of Caff decayed during GT oxidation [13–15]. The changes of GT secondary metabolites [14] and phenolics/quality potential of crush, tear, and curl BT [15] were reported during oxidation. The EGCg attenuated lipopolysaccharide (LPS)-induced nitric oxide (nitrogen monoxide, NO) production in cells [16]. The antiviral role of GTCs was reviewed [17]. The EGCg was identified as an inhibitor of phosphoglycerate mutase 1 (PGAM1) [18]. Quantitative analysis of GTCs from GT extract in human plasma was performed via UHPLC-MS [19].

The model is an expansion of solvent-dependent conformational analysis program (SCAP) from 1-octanol/water to other organic solvents [20]. In earlier publications, SCAP was used to compute the partition coefficients of porphyrins, phthalocyanines, benzobisthiazoles, fullerenes, acetanilides, local anesthetics (procaine analogues) [21], enzyme lysozyme [22], barbiturates, hydrocarbons (HCs) [23], polystyrene (PS) [24], Fe/S proteins [25], C-nanotubes (CNTs) [26], D-glucopyranoses, polyiodides, polyiodines, and crown ethers [27]. *Bioplastic evolution* (BPE) and quantitative structure-property relationships (QSPRs) were used for phenylalcohols, 4-alkylanilines [28], aromatics [29], phenylureas [30], pesticides [31], flavonoids [32], isoflavonoids [33], natural sesquiterpene lactones (STLs) [34], coffee chlorogenic acids (CGAs) [35], purine derivative alkaloid methylxanthines (Caff and its metabolites), alkaloid and predominant nicotine metabolite cotinine [36, 37], and tea leaf infusions [38]. Mucoadhesive polymer hyaluronan (HA) favors transdermal penetration absorption of model drug Caff [39, 40]. The present report explains QSPR examination and calculation of the retentions of tea compounds. The aim of this work is to discover features that differentiate tea components consistent with retentions. This study uses molecular descriptors

(MDs) for tea components. The goal is the corroboration of the values of MDs via their ability to distinguish tea phytochemicals, and their advantage as prognostic MDs for retention, contrasted with formation enthalpy, molecular weight, hydrophobic accessible surface (HBAS) area and partition. Section 2 describes the method. Sections 3 and 4 illustrate and discuss the results. Finally, the last section summarizes our conclusions.

2. Computational method

Biology presents an important idea ever elucidated in 400 years of experimental science: biological evolution (the other is the existence and organization of the periodic table of the elements). In *allometry* (biological scaling), *biological plastic* (*bioplastic*) *evolution* presents a viewpoint in evolutionary science. It conjugates the result of (1) the acquired characters and (2) associations rising between three rules: *evolutionary indeterminacy*, *morphological determination*, and *natural selection*. The association between morphology and functionality in the living forms stretches out in that the former is the substance foundation of the latter, which is the dynamic result of the former in the background of the relationship between the substantial setting and living substance. Morphology, functionality, energy cost, and vital viability are jointly affected: When a morphology is useful, it achieves its effort with least power charge, and the fundamental feasibility of the organ/organism is the utmost. Counting ideas engage describing *functional co-ordination index* I_c: the relationship between the work achieved by morphology T and the corresponding *morphological index* I_m:

$$I_c = T/I_m \tag{1}$$

The greater the work T attained by a specific morphology I_m, the greater the I_c. For an organism, Ruiz-Bustos suggested I_m as the relationship between morphological surface area S and body weight W [41]:

$$I_m = S/W \tag{2}$$

The replacement of Eq. (2) in Eq. (1) turns out to be

$$I_c = T/(S/W) = W \cdot T/S \tag{3}$$

The equation of T by its correspondence in classical mechanics provides

$$T = W \cdot x \cdot d^2x/dt^2 \tag{4}$$

Replacing Eq. (4) in Eq. (3) gives

$$I_c = W^2 \cdot x \cdot d^2x/\left(S \cdot dt^2\right) \tag{5}$$

The I_c rises as follows. (1) The greater the body weight at the same journeyed time/space, the greater the I_c. (2) The I_c is proportional to the gap journeyed in the shortest achievable time. (3) The smaller the body surface, the greater the I_c and function-morphology co-ordination needs lesser power charge.

Code SCAP is founded on an algorithm by Hopfinger, parametrized for 1-octanol and water solvents. One can center a *solvation sphere* on every group of the molecule [42, 43]. The intersecting volume V^o between the solvation and the van der Waals (VDW) spheres of the other atoms is computed. The SCAP handles four parameters for a solvent: (1) n: utmost number of solvent molecules filling the

solvation sphere; (2) Δg^{o}: change of the Gibbs free energy connected with the removal of one solvent molecule out of the solvation sphere [44, 45]; (3) R_v: radius of the solvation sphere; (4) V_f: *free volume* available for a solvent molecule in the solvation sphere. In this, part of the volume keeps out the solvent molecules. The volume contains the VDW volume of the group at which the sphere is centered and a volume on behalf of the groups bonded to the central one. The latter is modeled by a set of cylinders. The dissimilarity between the total volume of the solvation sphere and that excluded to the solvent molecules stands for volume V', which is accessible for n solvent molecules. The V_f is computed as $V_f = V'/n - V_s$. Variation of free energy, connected with the removal of all solvent molecules out of the solvation sphere of a group R, results in $\Delta G_R{}^{o} = n\Delta g^{o}\ (1-V^{o}/V')$ and the solvation free energy of a molecule $\Delta G_{solv^{o}} = -\Sigma_{R=1}{}^{N}\Delta G_R{}^{o}$. The partition coefficient P between 1-octanol and water results in

$$RT\ln P = \Delta G^{o}_{solv}(\text{water}) - \Delta G^{o}_{solv}(\text{1-octanol}) \tag{6}$$

at a given temperature T taken as 298 K, where R is the gas constant and $\Delta G_{solv^{o}}$ (1-octanol) and $\Delta G_{solv^{o}}$ (water) the standard-state Gibbs free energies of solvation in kJ·mol^{-1}. Extending SCAP for dissimilar solvents, the parameters were adapted, considering the result of relative permittivity and molecular volume on 1-octanol properties. For a general solvent, the utmost number of solvent molecules, which permitted packing the solvation sphere, is connected with the molecular volume of the solvent as follows:

$$n_s = n_o(V_s/V_o)^{\log\frac{n_o}{n_w}/\log\frac{V_o}{V_w}} \tag{7}$$

where V_o, V_w, and V_s are the molecular volumes of 1-octanol, water, and general solvent, respectively. The n_o, n_w, and n_s are the utmost numbers of molecules of 1-octanol, water, and general solvent, respectively, which allowed packing the solvation sphere. The change in the standard Gibbs free energy is connected with the removal of one solvent molecule out of the solvation sphere, $\Delta G_S{}^{o}$, which is computed via the generalized Born equation

$$\Delta g^{o}_s = \Delta g^{o}_o(1-1/\varepsilon_s)/(1-1/\varepsilon_o) = \Delta g^{o}_o\varepsilon_o(\varepsilon_s-1)/[\varepsilon_s(\varepsilon_o-1)] \tag{8}$$

where $\Delta g_o{}^{o}$ denotes Δg^{o} for 1-octanol, and ε_o and ε_s are the relative permittivities of 1-octanol and general solvent. The radius of the solvation sphere is connected with the molecular volume of the solvent molecule as follows:

$$R_{v,s} = R_{v,o}(V_s/V_o)^{1/3} \tag{9}$$

where $R_{v,o}$ denotes R_v for 1-octanol. The free volume accessible for a solvent molecule in the solvation sphere is as follows:

$$V_{f,s} = V_{f,o}V_s/V_o \tag{10}$$

where $V_{f,o}$ denotes V_f for 1-octanol.

3. Calculation results

For the 12 tea components {polyol acids [quinic (*cf*. **Figure 1a**) and coumaroylquinic acids (**Figure 1h**)], non-flavonoid polyphenols [gallic acid

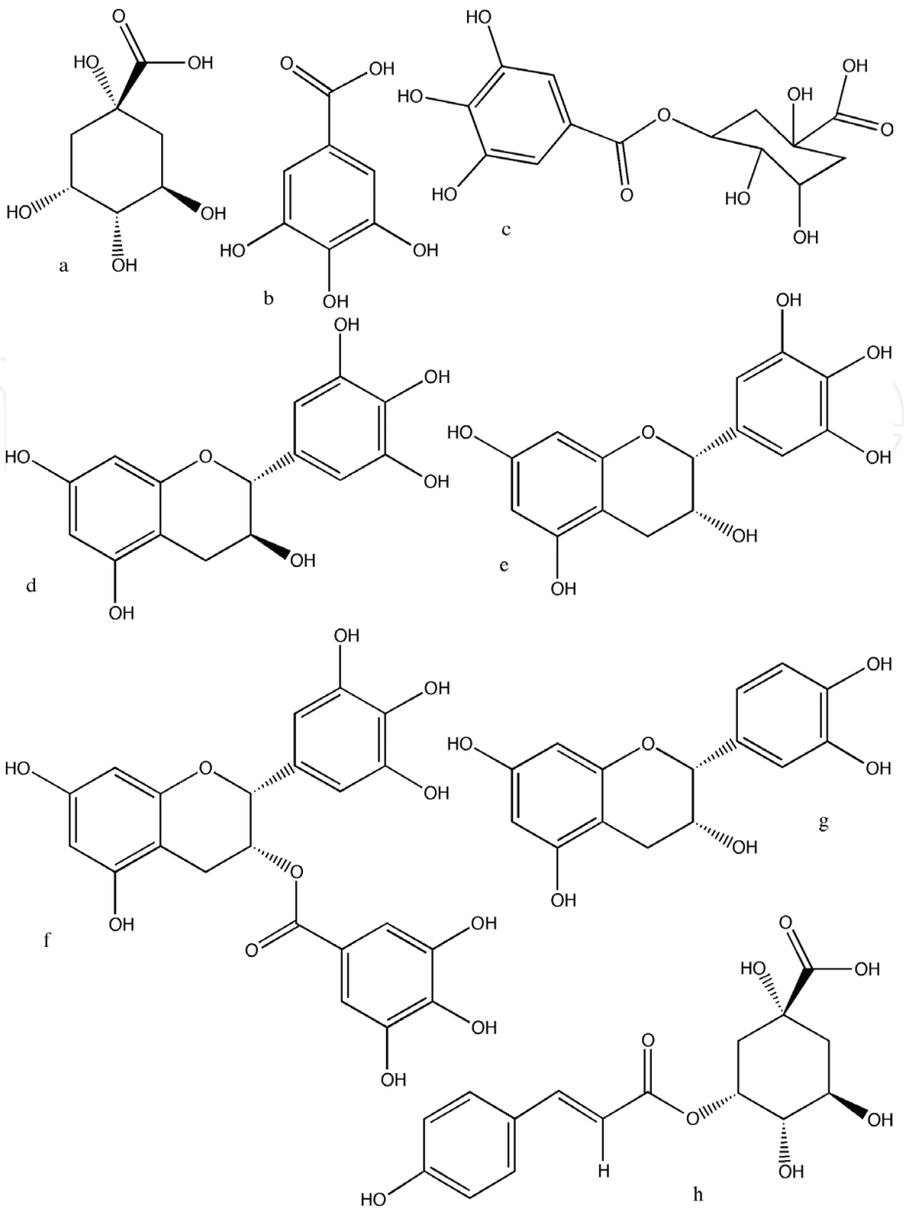

Figure 1.
(a) Quinic acid, (b) gallic acid, (c) theogallin, (d) GC, (e) EGC, (f) EGCg, (g) EC, and (h) coumaroylquinic acid.

(**Figure 1b**) and corilagin], glycosides [theogallin (**Figure 1c**), digalloyl glucose, and trigalloyl glucose] and GTCs [GC (**Figure 1d**), EGC (**Figure 1e**), EGCg (**Figure 1f**), EC (**Figure 1g**), and ECg]}, UHPLC retention times, R_t, were obtained by Barsch et al. *Epi*-diastereoisomers show the gallate, etc. residues in *cis*-position. The chromatographic analysis is in accord with the technical literature [46].

Quinic acid was taken as the reference molecule for the retention time R_t^o, owing to its least R_t (*cf*. **Table 1**). Relative changes $(R_t–R_t^o)/R_t^o$ were computed for all the components. The molar formation enthalpy was calculated with code MOPAC-AM1 [47]. The diastereoisomers GC and EGC show similar formation enthalpy and HBAS. Decaffeination does not alter the metabolite composition extensively. Caffeine does not differentiate the samples since the data were acquired in ESI NI mode where Caff does not ionize.

In molecular structures, the use of co-ordination MDs needs adapting variables T, S, and W (Eq. (3)): T is redescribed as minus standard formation enthalpy ($kJ·mol^{-1}$); S, molecular surface area ($Å^2$); and W, molecular weight ($g·mol^{-1}$). The MDs of the tea components (*cf*. **Table 2**) illustrate that I_m is constant, while I_c rises

with *W*. The molecular surface and HBAS areas were computed with our code TOPO [48]. The diastereoisomers, GC and EGC, show similar physico/physiochemical features and BPE MDs.

Molecule	R_t (min)	$R_t - R_t°$ (min)	$(R_t - R_t°)/R_t°$	$\Delta H_f°$ (kJ·mol^{-1})[a]	HBAS (Å^2)[b]
Quinic acid	0.8	0.0	0.000	−1239.5	89.68
Gallic acid	2.4	1.6	2.000	−836.0	85.88
Theogallin	2.8	2.0	2.500	−1773.2	130.20
Gallocatechin (GC)	3.5	2.7	3.375	−1078.1	173.11
Corilagin	4.9	4.1	5.125	−2722.5	233.83
Epigallocatechin (EGC)	5.0	4.2	5.250	−1063.5	174.31
Digalloyl glucose	5.3	4.5	5.625	−2362.3	223.46
Epigallocatechin gallate (EGCg)	6.0	5.2	6.500	−1590.7	209.50
Epicatechin (EC)	6.4	5.6	7.000	−880.4	202.04
Coumaroylquinic acid	6.7	5.9	7.375	−1372.0	265.79
Trigalloyl glucose	6.9	6.1	7.625	−2908.9	291.39
Epicatechin gallate (ECg)	7.0	6.2	7.750	−1434.9	260.13

[a]*Molar formation enthalpy calculated with MOPAC–AM1.*
[b]*HBAS: hydrophobic solvent-accessible surface area (Å^2).*

Table 1.
Retention, formation enthalpy, and hydrophobic-accessible surface area for tea components.

Molecule	*W* [g·mol^{-1}][a]	*T* [kJ·mol^{-1}][b]	*S* [Å^2][c]	I_m [mol·Å^2·g^{-1}][d]	I_c [kJ·g·mol^{-2}·Å^{-2}][e]
Quinic acid	192	1239.5	196.08	1.021	1213.7
Gallic acid	170	836.0	168.23	0.990	844.8
Theogallin	344	1773.2	322.48	0.937	1891.5
Gallocatechin (GC)	306	1078.1	285.27	0.932	1156.4
Corilagin	634	2722.5	518.71	0.818	3327.6
Epigallocatechin (EGC)	306	1063.5	286.51	0.936	1135.8
Digalloyl glucose	484	2362.3	421.88	0.872	2710.1
Epigallocatechin gallate (EGCg)	458	1590.7	410.89	0.897	1773.1
Epicatechin (EC)	290	880.4	274.36	0.946	930.6
Coumaroylquinic acid	338	1372.0	332.68	0.984	1393.9
Trigalloyl glucose	636	2908.9	550.91	0.866	3358.2
Epicatechin gallate (ECg)	442	1434.9	401.04	0.907	1581.5

[a]*W: molecular weight (g·mol^{-1}).*
[b]*T: minus standard formation enthalpy (kJ·mol^{-1}).*
[c]*S: molecular surface area (Å^2).*
[d]*I_m: morphological index (mol·Å^2·g^{-1}).*
[e]*I_c: co-ordination index (kJ·g·mol^{-2}·Å^{-2}).*

Table 2.
BPE indices for the compounds of tea extracts.

In the plot of MDs vs. molecular weight W (*cf*. **Figure 2**), some points collapse, especially diastereoisomers GC and EGC with similar BPE MDs. The only index that is constant is I_m. The MDs are more responsive to W decay: $I_c > T > S > I_m$.

Changes in $(R_t–R_t^o)/R_t^o$ vs. molar formation enthalpy ΔH_f^o and molecular weight M_w present correlation. The model is

$$\left(R_t - R_t^o\right)/R_t^o = 1.10 + 0.00484\Delta H_f^o + 0.0304M_w, n = 12\, r = 0.833$$
$$s = 1.540\ \ F = 10.2\ \ \text{MAPE} = 21.66\%\ \ \text{AEV} = 0.3064 \qquad (11)$$

where r is the correlation coefficient, s, the standard deviation, and F, the Fisher ratio. The mean absolute percentage error (MAPE) is 21.66% and the approximation error variance (AEV) is 0.3064. The addition of the co-ordination MD I_c betters the fit

$$\left(R_t - R_t^o\right)/R_t^o = -0.218 + 0.0348M_w - 0.00456I_c, n = 12\, r = 0.864$$
$$s = 1.403 \quad F = 13.2 \quad \text{MAPE} = 20.47\%\ \ \text{AEV} = 0.2543 \qquad (12)$$

and AEV decays by 17%.

Adding the quadratic hydrophobic solvent-accessible surface area betters the fit

$$\left(R_t - R_t^o\right)/R_t^o = 0.654 + 0.0153M_w - 0.00260I_c + 0.0000738\text{HBAS}^2,$$
$$n = 12\ \ r = 0.954\ \ s = 0.887\ \ F = 26.9$$
$$\text{MAPE} = 12.33\%\ \ \text{AEV} = 0.0922 \qquad (13)$$

and AEV decays by 70%. The integration of the molar formation enthalpy improves the fit, according to lesser standard deviation, greater Fisher statistic, and lesser AEV:

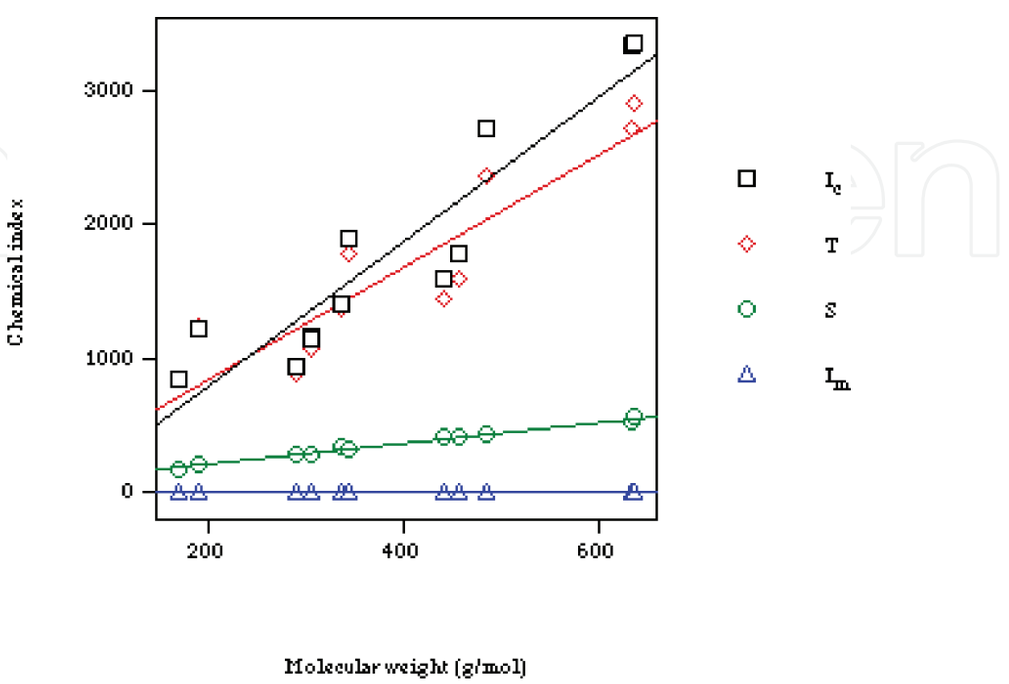

Figure 2.
Variation of chemical indices for tea compounds vs. molecular weight: y = −300 + 5.42x; y = −10.3 + 4.21x; y = 51.2 + 0.773x; y = 1.06–0.000352x.

$$\left(R_t - R_t^o\right)/R_t^o = 1.45 + 0.00279\Delta H_f^o + 0.0121M_w + 0.0000806\text{HBAS}^2,$$
$$n = 12\, r = 0.954\, s = 0.881\, F = 27.2\ \text{MAPE} = 12.57\%$$
$$\text{AEV} = 0.0912 \tag{14}$$

and AEV decays by 70.2%. The formation enthalpy and hydrophobic-accessible surface better the fit

$$\left(R_t - R_t^o\right)/R_t^o = -1.24 + 0.00111\Delta H_f^o + 0.0412\text{HBAS}, n = 12$$
$$r = 0.956\, s = 0.820\, F = 47.3\ \text{MAPE} = 11.97\%$$
$$\text{AEV} = 0.0868 \tag{15}$$

and AEV decays by 72%. The quadratic logarithm of the 1-octanol/water partition coefficient improves the fit

$$\left(R_t - R_t^o\right)/R_t^o = -1.44 + 0.00187\Delta H_f^o + 0.0452\text{HBAS} + 0.0149(LogP)^2,$$
$$n = 12\, r = 0.959\, s = 0.836\, F = 30.6\ \text{MAPE} = 11.64\%$$
$$\text{AEV} = 0.0807 \tag{16}$$

and AEV decays by 74%. However, this development should be taken with care because though the correlation coefficient, MAPE, and AEV enhance (greater r, and lesser MAPE and AEV), the standard deviation and Fisher statistic deteriorate (greater s and lesser F) because of one less degree of freedom in the model: notice three vs. two variables in Eqs. (16) and (15), respectively. Linear equations (11), (12), and (15) are more satisfactory for extrapolation than quadratic equations (13), (14), and (16), which go better with intrapolation. Extra fitting parameters were tested: molecular dipole moment, organic solvent/water partition coefficients, free energies of solvation and transfer from water to organic solvents, molecular volume, surface area, globularity, rugosity, hydrophilic (HLAS) and total solvent-accessible surface (AS) areas, molecular fractal dimension, and fractal dimension averaged for external atoms. Notwithstanding, the results do not better Eqs. (11)–(16).

4. Discussion

Molecular studies allowed predicting parameters related to phytochemicals, drugs, and metabolite bioactivities. Direct correlation of MDs with activity was obtained. The chromatographic behavior of drugs in phases of different polarity contains information about their pharmacological performance, e.g., barbiturates and neuroleptics. Chromatographic parameters in a polar stationary phase system correlate better with some MDs, whereas Kováts parameters, obtained from the apolar phase interaction, correlate the best with some others. The MDs predict chromatographic parameters, e.g., retention times in gas chromatography (GC)/LC and retention factor R_f in thin-layer chromatography (TLC). Topological MDs (TDs) were used in chromatographic chiral separations. The chromatographic properties of natural phenol/sugar derivatives were predicted by molecular topology (MT). The properties of chiral quinic acid, theogallin, (+)-GC, (−)-EGC, digalloyl glucose, (−)-EGCg, (−)-EC, trigalloyl glucose, and (−)-ECg were forecasted by MT.

This study related LC-MS retentions for tea compounds to MDs. Molecular functions were obtained through multivariate linear (MVLR) and quadratic (MVQR) regressions, which were selected based on their statistical parameters. Regression

analysis of the molecular functions showed a forecast of the experimental elution sequence for the tea components. In order to predict the sequence in tea substances, two- or three-variable models were used in which the appearance of the co-ordination index, molar formation enthalpy, molecular weight, HBAS, or 1-octanol/water partition coefficient reveals the importance of thermodynamic, *steric*, geometric, and lipophilic analysis in retention, allowing the use of such equations in predicting its value. Molecular structures may be differentiated even in other derivatives of tea components not included in the series. Weak MVQR relationships appeared between physico/physiochemical properties (log*P* and HBAS) and retention.

The reason why plants accumulate polyphenols is related to their defense system, and their functions depend on chemical reactivity and physico/physiochemical properties. The structural diversity of plant polyphenols in nature indicates that they present different and wide-ranging functions. Some polyphenols, e.g., GTCs and proanthocyanidins, are susceptible to enzymatic and nonenzymatic oxidation depending on the plant. Polyphenol oxidation in plant tissues, e.g., BT production, proceeds with a reduction in oxygen molecules or polyphenol quinines, in which reactivity with proteins and other co-existing compounds plays a role during postharvesting. The secondary polyphenols, produced in plants after physical tissue damage, relate to the plant defense system though many products were not characterized chemically. Artificial processing, e.g., drying, oxidation, and roasting, is different from the natural reactions, e.g., insolubilization and polymerization, occurring in living plants and produces different compounds. Scientific studies indicated that polyphenols in foods present health benefits. Identifying the mechanisms of their production and chemical structures is important. The GT presents the greatest variability in physico/physiochemical properties. Many beneficial effects of GT are related to GTCs, particularly ECg and, especially, EGCg content. The BBB permeability, easy access via the diet, and low toxicity show them as promising molecules, for prevention and treatment of chronic neurodegenerative diseases.

5. Conclusion

From the discussion of the present results, the conclusions follow.

1. The object of this work was to build up structure-property relationships for the qualitative and quantitative calculation of the ultrahigh-performance liquid chromatographic retention times of tea components. The outcomes add an augmented scientific knowledge in the field of association calculation of components in dissimilar tea samples.

2. Structure-property relationships result as expected for predicting retention times, for the elucidation of unknown components in metabolomics studies. Code SCAP permits the hydration and solvation free energies, and partition coefficients, which show that for a given atom, energies and partition coefficients are responsive to the occurrence in the molecule of other atoms and functional groups.

3. The parameters needed to compute the co-ordination descriptor are the molar formation enthalpy, molecular weight, and surface area. Linear and quadratic correlation models were obtained for the chromatographic retention time.

4. A benefit of our structure-activity relationships is that they discover feeble quadratic relationships, occurring between the partition coefficient,

hydrophobic solvent-accessible surface area, and retention. The tendency between the co-ordination index and the molecular weight indicates not only a homogeneous molecular structure of tea components but also the capacity to calculate and adapt their features, which is nontrivial in metabolomics studies.

5. The result of dissimilar kinds of characteristics was examined: thermodynamic, *steric*, geometric, lipophilic, etc. The molar formation enthalpy, molecular weight, hydrophobic solvent-accessible surface area, partition coefficient, etc. differentiated tea components in linear and quadratic equation models.

6. The morphological and co-ordination descriptors completed multivariable regression expressions for the chromatographic retention.

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Conflict of interest

The authors declare no conflict of interest.

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