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RESEARCH ARTICLE

Assessment of medicinal tree diversity in the Chintamoni Kar Bird Sanctuary (CKBS), Kolkata, India and prediction of antimutagenic phytochemicals by using software

Pamela Banerjee and Soumendra Nath Talapatra*

Career Advancement Solutions, H2 – 120A/New Bener Pole Road, Maheshtala, Kolkata 700141, India

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Corresponding Author

Soumendra Nath Talapatra

Abstract

The study of bioactive chemicals containing medicinal trees diversity is an important research work. These organics provide knowledge about phytochemicals from natural origin, which protect against several diseases, mutagenesis and carcinogenesis. These natural chemical ingredients may be used as antimutagenic potential. The present study aims to know the qualitative and quantitative assessment of common medicinal tree diversity located at Chintamoni Kar Bird Sanctuary (CKBS), Kolkata, India and study of various literatures also to know phytochemicals present in their different parts and to predict mutagenicity or antimutagenicity through QSAR modeling T.E.S.T. software of these phytochemicals. The results clearly indicated that there were 11 types of tree species and the total populations were 93 nos. in the study area. Many literatures clearly revealed that these plants as a whole and/or their parts have potent phytochemicals to prevent mutagenicity and these phytochemicals have already been studied as antimutagenic in nature. Among all these phytochemicals 4 polyphenols types viz. epigallocatechin gallate, quercetin, zeatin and ellagic acid and skimmianine alkaloid were predicted mutagenic compounds while other polyphenols viz. catechin, flavonol, rutin, phenolic acid, lupeol, coumarin, psoralen, bergapten, kaempferol, friedelin, gallic acid, chlorogenic acid, vanillic acid and ferulic acid and other sterols like β-sitosterol, were predicted antimutagenic compounds. In conclusion, present work was emphasized that antimutagenic tree species in the study area should be conserved for their natural chemical ingredients. Therefore, biodiversity study, phytochemicals estimation as antimutagens and conservation of these particular tree species in different common areas might be relevant in relation to prevent mutagenesis and carcinogenesis.

INTRODUCTION

Medicinal plants generate naturally bioactive compounds viz. phenolic compounds including flavonoids, alkaloids, sterols etc. that have power of protection against diseases. The plants have been used as medicines through traditional knowledge (Chantia, 2003; Lal and Singh, 2012; Sinhababu and Banerjee, 2013). Natural bioactive compounds from different plants are of particular importance because they are preventive for carcinogenesis (Sanjib, 2011), antigenotoxic (Talapatra et al., 2010) and also protect from hyperglycemia, malaria, liver dysfunction, dysentry, inflammations, anal hemorrhoids, lung and kidney diseases, antimicrobial (antifungal and antibacterial), antiulcer, insnomia, antifertility /contraception, hypotensive, wound healing etc. (Ahmed and Urooj, 2010; Ramila Devi and Manoharan, 2011; Shivalinge and Vrushabendra, 2011; Barangi et al., 2012; Satish et al., 2013; Shad et al., 2014; Das et al., 2015).

It has been suggested that regular eating of anticarcinogens and antimutagens in the diet may be the most effective way of preventing human carcinogenesis and search for novel antimutagens acting in chemoprevention through phytochemicals (Gowri and Chinnaswamy, 2011). Biodiversity study has been postulated that species distributed surrounding cities, potentially due to variation in plant specis at micro level alongwith other biological resources (Turner et al., 2007).

Quantitative Structure Activity Relationships (QSARs) are easy screening mathematical models, which are used to predict measures of toxicity/mutagenicity as end point in test models from physical characteristics of the structure of chemicals by using suitable 2-dimensional and 3-dimensional molecular descriptors. According to Choplin (2005) and Valentina et al. (2009), the molecular descriptors are used on the basis of three parameters called as thermodynamic, steric and electronic in QSAR modeling. It was already established that QSAR modeling is one of the basic tools of modern drug and pesticide design, study of endpoints viz. toxicity, mutagenicity etc. in science (Hansch and Leo, 1995; Franke and Gruska, 2003; Benigni, 2005; Talapatra et al., 2015). Carcinogenesis and mutagenesis are among the toxicity endpoints that pose the great concern. Moreover, to prevent these impacts, potent phytochemicals have been established and easy prediction of these bioactive compounds whether antimutagenic and mutagenic, can be predicted through QSAR modeling T.E.S.T. (Toxicity Estimation Software Tool) software (USEPA, 2012). It was documented that common tree species have potent chemicals for medicinal usage (Agarwal and Pandey, 2009; Satwinderjeet et al. 2010; Sanjib, 2011; Satish et al., 2013; Espanha et al., 2014; Joselin et al., 2014). Various studies from four decades have been established in order to identify compounds, which might be antigenotoxic especially prevent DNA-damage and its consequences in organisms (de Flora and Ramel, 1988). Many bioactive compounds extracted from plant species are known as antimutagens and thus have a full range of prospective applications in human healthcare especially mutagenesis and carcinogenesis (Satish et al., 2013). The plant diversity study for avenues, peripheral afforestation, parks, suburbs etc. have already been documented nationally and internationally (Benthal, 1946; Chakraverty and Jain, 1984; McPherson and Rowntree, 1989; Galvin, 1999; Mukhopadhyay and Chakraverty, 2008; Zainudin et al., 2012; Talapatra, 2013; Das et al., 2015) but no one has reported to study the diversity of medicinal trees found in CKBS, Kolkata, India and known phytochemicals from literatures study along with the easy screening of potent antimutagenic compounds by using QSAR modeling T.E.S.T. software (USEPA, 2012).

The present study aims to know the qualitative and quantitative assessment of common medicinal tree diversity located at CKBS, Kolkata, India and study of various literatures for phytochemicals present in their different parts and also to predict whether these compounds are mutagenic or antimutagenic through QSAR modeling by using T.E.S.T. software.

MATERIALS AND METHODS

The study area was selected at Koyler Bagan or Chintamoni Kar Bird Sanctuary or CKBS (latitude = 22° 25´ N and longitude = 88° 24´ E), Kolkata, India. The field study was carried out in the month of January 2015 (winter season). The qualitative and quantitative study was done by 900 meter line transect and the medicinal tree species variety and individual number of species was calculated as described by the methods of Jaenson et al. (1992). Field study was done by variety and counting the plant species and visual identification and finally image capture in this study. The diversity of plant species were studied by qualitative and quantitative assessment as chemotherapeutic species. The usage of parts of the plants and their bioactive compounds as phytochemicals were studied and tabulated from various literatures already established by many researchers.

The prediction of Ames mutagenicity test for common available phytochemicals was carried out by using T.E.S.T. software Ver 4.1. It was predicted mutagenic or antimutagenic that organic compounds found in present tree species as reviewed from various literatures. It was reported that T.E.S.T. software package estimates mutagenicity using a variety of QSAR methodologies viz. hierarchical clustering, the Food and Drug Administration (FDA) MDL, nearest neighbor and a consensus, which is simply the average of the predicted from other QSAR methodologies, based on the applicability domain for each method (Zhu et al., 2009). Particular chemical structure can easily be visualized after entering CAS no in T.E.S.T. According to User's guide (USEPA, 2012), it was reported for the Ames test, frame-shift mutations or base-pair substitutions can only be occurred for any test chemical when exposed to histidine-dependent strains of *Salmonella typhimurium*. It was known when strains are exposed to a mutagen, reverse mutations occurred by the functional ability of the bacteria to synthesize histidine dependent bacterial colony growth on the histidine deficient medium, called revertants. The compound is classified Ames positive when it

induced revertant colony growth in any one of out of five strains. In the T.E.S.T. a dataset of 6512 chemicals was compiled by Hansen and coworkers from several different sources (Hansen et al. 2009). The final dataset consists of 5743 chemicals (after excluding salts, mixtures, ambiguous organics and compounds having unavailable CAS numbers). For external statistical validation, the consensus method was achieved the best prediction accuracy (concordance) and prediction specificity (USEPA, 2012). The single model and group contribution methods could not be applied to this endpoint and all of the methods achieved a nice balance of prediction on the basis of concordance (accuracy), sensitivity and specificity (USEPA, 2012).

The study of predictive mutagenicity or antimutagenicity of natural phenolic compounds including flavonoids and others like steroids, xanthones and alkaloids in studied tree species. A QSAR study was carried out in this work with the aim to obtain mathematical models by using T.E.S.T software that could be used and easily to know predicted values for mutagenic or antimutagenic by Ames mutagenicity test.

RESULTS

The present results clearly indicate that qualitative and quantitative diversity of plants in the park known as CKBS and their parts contain potent medicinal properties along with antimutagenic and anticarcinogenic properties as phytochemicals after studying from various literatures (Table 1). There are 11 types of trees were found in the studied area. These species are *Ficus racemosa* (45 nos), *Mangifera indica* (25 nos), *Ficus bengalensis* (2 nos), *Moringa oleifera* (3 nos), *Hibiscus mutabilis* (1 no), *Artocarpus heterophyllus* (2 nos), *Ziziphus jujube* (1 no), *Aegle marmelos* (1 no), *Annona squamasa* (2 nos), *Cocos nucifera* (10 nos) and *Euphoria longan* (1 no).

Table 2 was showed predicted results of mutagenic and antimutagenic properties of polyphenols, flavonoids, sterols and alkaloids found in different parts of trees. 25 types of polyphenols including flavonoids viz. catechin, quercetin-3-D-galactoside, flavonol, rutin, phenolic acid, epigallocatechin gallate, lupeol, coumarin, quercetin, psoralen, bergapten, caffeoylquinic acid, kaempferol, friedelin, tannin, zeatin, saponin, pro-anthocyanidin A2, (-)-epicatechin, gallic acid, ellagic acid, chlorogenic acid, vanillic acid, ferulic acid and β-carotene were studied and 3 types of sterols viz. β-sitosterol, taraxasterol and terpenoid were also studied and 1 type of C-glucosylxanthone or mangiferin as xanthones and 2 types of alkaloids such as aegeline and skimmianine were studied.

Among all these phytochemicals 4 polyphenols types viz. epigallocatechin gallate (0.90), quercetin (0.55), zeatin (0.67) and ellagic acid (0.67) and skimmianine alkaloid (0.90) were predicted mutagenic positive (+) compounds while other polyphenols viz. catechin (0.46), flavonol (0.19), rutin (0.06), phenolic acid (0.05), lupeol (0.19), coumarin (0.30), psoralen (0.49), bergapten (0.24), kaempferol (0.39), friedelin (0.12), gallic acid (0.31), chlorogenic acid (0.19), vanillic acid (-0.09), ferulic acid (0.22) and β-carotene (-0.01) and other sterols viz. β-sitosterol (0.25) were predicted antimutagenic or mtagenic negative (-) compounds. Polyphenols such as quercetin-3-D-galactoside, caffeoylquinic acid, tannin, saponin, pro-anthocyanidin A2, (-)-epicatechin and sterols like taraxasterol and terpenoid and xanthones like C-glucosylxanthone or mangiferin were unable to predict due to unavailability of CAS no. matching in the software (Table 2). It was found the established data for experimental mutagenicity test in T.E.S.T. software, the polyphenols viz. coumarin, quercetin, bergapten, kaempferol and β-carotene and also skimmianine alkaloid were mutagenic positive (+) and the value was observed 1.00 for all these 6 compounds while other polyphenols like psoralen, gallic acid, ellagic acid, chlorogenic acid, ferulic acid and sterols like β-sitosterol were showed mutagenic negative (-) value. The experimental data for rest polyphenols viz. catechin, flavonol, rutin, phenolic acid, epigallocatechin gallate, lupeol, friedlin, zeatin and vanillic acid were not available in this software (Table 2).

It was found that the software predicted on the basis of statistical external validation by calculating external test set and training set alongwith appropriate inbuilt molecular descriptors. The prediction value was found as per best accuracy (concordance value) alongwith prediction sensitivity and specificity. It was observed that highest percentage in concordance, sensitivity and specificity values determined the test chemical was present in the training set and the prediction does not represent an external prediction. It was defined in software that if similar test set chemicals were predicted well in relation to the entire test set, it has higher confidence in the predicted value for external test set and if the predicted value matches the experimental values for similar compounds in the training set then similar compounds will be predicted well, it has also higher confidence in the predicted value (Table 2). The cluster FDA model fit results were observed in the T.E.S.T. software through statistical data prediction for concordance (accuracy), sensitivity and specificity and also model coefficient with equation for individual data were tabulated and expressed in Table 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20 and 21 except lupeol and friedelin due to unavailability in software.

Table 1. Qualititaive and quantitative assessment of medicinal trees located in CKBS, Kolkata and their therapeutic values as per literatures

Sl. No.	Plant species (common name)	Plant species (scientific name)	No. of individual species	Part (s) used	Researches done on phytochemicals	Disease prevention	Literatures Referred
1.	Cluster fig	*Ficus racemosa*	45	Fruit, stem bark	Coumarin, tannins and glutathione	diabetes, liver disorders, diarrhea, inflammatory conditions, hemorrhoids, respiratory, and urinary diseases	Ahmed and Urooj, 2010; Ramila Devi and Manoharan, 2011; Shivalinge and Vrushabendra, 2011; Barangi et al., 2012
2.	Mango	*Mangifera indica*	25	Stem bark, leaf, fruit	Catechin, epigallocatechin gallate, flavonoids, glycosides, xanthone derivatives and C-glucosylxanthones (mangiferin)	antidiuretic, antidiarrheal, antiemetic and cardiac	Yoshimi et al., 2001; Rodriguez et al., 2006 Aqil et al., 2006 Barreto et al., 2008
3.	Banyan	*Ficus bengalensis*	02	Stem, bark and fruit	Flavonol, rutin, friedelin, taraxosterol, lupeol, b-amyrin, psoralen, bergaptenand β-sisterol, quercetin-3-D-galactoside	antidiabetic, antiinflammatory, antitumoractivity, anticancer, cytoprotective and antiulcer activity, antinociceptive, antioxidant, hypolipidemic, antihyperglycemic, and antipyretic.	Satish et al., 2013 Sharma et al., 2009
4.	Drumstick	*Moringa oleifera*	03	Leaves, roots, seed, bark, fruit, flowers and immature pods	Thiocarbamate, isothiocyanate glycosides, tanin, flavonoids, zeatin, quercetin, β-sitosterol, caffeoylquinic acid, kaempferol, β-carotene	cardiac and circulatory stimulants, antitumor, antipyretic, antiepileptic, antiinflammatory, antiulcer, antispasmodic, diuretic, antihypertensive, cholesterol lowering, antioxidant, antidiabetic, hepatoprotective, antibacterial and antifungal	Anwar et al., 2007; Satish et al., 2013
5	Land lotus	*Hibiscus mutabilis*	01	Leaf and flower	Flavonoids (rutin, Kamferol, quercetin)	emollient and cooling, and are used to treat swellings and skin infections	Dasuki, 2001; Kurian et al., 2012
6.	Jackfruit	*Artocarpus heterophyllus*	02	Fruit, seed, latex	Phenolic compounds, flavonoids, sterols	antioxidant, antiinflammatory, antibacterial, anticariogenic, antifungal, antineoplastic, hypoglycemic, wound healing	Baliga et al., 2011; Bacayo et al., 2012
7.	Ber	*Ziziphus jujube*	01	Fruit	Polyphenols, flavonoids, alkaloids, terpenoids and saponins.	antifungal, antibacterial, antiulcer, sedative, antiinlammatory, antispastic, antifertility /contraception, hypotensive, wound healing	Shad et al., 2014
8.	Bel / Wood apple	*Aegle marmelos*	01	Leaves, root, fruit	Alkaloids (aegeline, skimmianine	gastro intestinal diseases, piles, oedema, jaundice, vomiting, obesity, pediatric disorders, gynecological disorders, urinary complaints and as a rejuvenative	Riyanto et al., 2001; Lanjhiyana et al., 2012

9.	Sitaphal / Custard Apple	*Annona squamasa*	02	Leaves, root bark, seeds	Steroid, terpeniod, glycoside, alkaloid, flavonid saponin and phenolic compounds and alkaloids	anticancer, antitumour, abscesses, insect bites, skin complaints, antibacterial, toothache, kill head-lice and fleas (seed powder should not contact with eyes), antimalarial	Saha, 2011
10.	Coconut	*Cocos nucifera*	10	Fruit endocarp	Phenolic (chlorogenic acid, vanillic acid and ferulic acid) and flavonoids (quercetin)	metabolic disorder, antioxidant, antimicrobial, vasorelaxant, antihypertensive, antioxidant	Singla, 2012
11.	Anshfall	*Euphoria longan*	01	Fruits edible, leaves and flowers	Polyphenols (pro-anthocyanidin A2, (-)-epicatechin, gallic acid and ellagic acid)	Antioxidant, antiinflamatory, antidiabetic, anticancer	Lin et al., 2012

Table 2. Prediction of mutagenic and antimutagenic phytochemicals by QSAR modeling software (T.E.S.T.)

Sl. No.	Phytochemicals	CAS No.	Ames Mutagenicity estimation	Ames Mutagenicity estimation by T.E.S.T (Consensus method)
			Experimental value*	Predicted value*
	Polyphenols			
1.	Catechin	154-23-4	N/A	0.46 (–)
2.	Quercetin-3-D-galactoside	482-36-0	n.f.	n.f.
3.	Flavonol	577-85-5	N/A	0.19 (–)
4.	Rutin	153-18-4	N/A	0.06 (–)
5.	Phenolic acid	122-03-2	N/A	0.05 (–)
6.	Epigallocatechin gallate	989-51-5	N/A	0.90 (+)
7.	Lupeol	545-47-1	N/A	0.19 (–)
8.	Coumarin	91-64-5	1.00 (+)	0.30 (–)
9.	Quercetin	117-39-5	1.00 (+)	0.55 (+)
10.	Psoralen	66-97-7	0.00 (–)	0.49 (–)
11.	Bergapten	484-20-8	1.00 (+)	0.24 (–)
12.	Caffeoylquinic acid	1241-87-8	n.f.	n.f.
13.	Kaempferol	520-18-3	1.00 (+)	0.39 (–)
14.	Friedelin	559-74-0	N/A	0.12 (–)
15.	Tannin	1401-55-4	n.f.	n.f.
16.	Zeatin	1637-39-4	N/A	0.67 (+)
17.	Saponin	8047-15-2	n.f.	n.f.
18.	Pro-anthocyanidin A2	41743-41-3	n.f.	n.f.
19.	(-)-Epicatechin	490-46-0	n.f.	n.f.
20.	Gallic acid	149-91-7	0.00 (–)	0.31 (–)
21.	Ellagic acid	476-66-4	0.00 (–)	0.67 (+)
22.	Chlorogenic acid	327-97-9	0.00 (–)	0.19 (–)
23.	Vanillic acid	121-34-6	N/A	-0.09 (–)
24.	Ferulic acid	1135-24-6	0.00 (–)	0.22 (–)
25.	β-carotene	7235-40-7	1.00 (+)	-0.01 (–)
Sterols				
1.	β-sitosterol	83-46-5	0.00 (–)	0.25 (–)
2.	Taraxasterol	1059-14-9	n.f.	n.f.
3.	Terpenoid	68917-63-5	n.f.	n.f.
Xanthones				
1.	C-Glucosylxanthone or mangiferin	4773-96-0	n.f.	n.f.
Alkaloids				
1.	Aegeline	456-12-2	n.f.	n.f.
2.	Skimmianine	83-95-4	1.00 (+)	0.90 (+)

*** = values are of revertant/plate; (–) = mutagenicity negative i.e. antimutagenic; (+) = mutagenicity positive i.e. mutagenic; n.f. = Not found and N/A = Not available in T.E.S.T. software**

Table 3. Statistical validation of FDA cluster model fit results for catechin

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.867 (26 out of 30)	0.857 (18 out of 21)	0.889 (8 out of 9)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	5.4265	4.2172

icycm	Total information on the vertex cycle matrix magnitude	0.0024	0.0014
BELe2	Lowest eigenvalue n. 2 of Burden matrix / weighted by atomic Sanderson electronegativities	-3.0003	2.2625

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.0024×(icycm) - 3.0003×(BELe2) + 5.4265**

Table 4. Statistical validation of FDA cluster model fit results for flavonol

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.943 (33 out of 35)	0.750 (6 out of 8)	1.000 (27 out of 27)	35

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-9.4956	5.0842
AMW	Average molecular weight	0.2510	0.1398
GATS7m	Geary autocorrelation - lag 7 / weighted by atomic masses	0.8064	0.3205
GATS4e	Geary autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	0.8258	0.5043
CID2	Average Randic Connectivity ID number	3.0130	2.4353
-CH< [aromatic attach]	-CH< [aromatic attach] fragment count	-0.2505	0.2302

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.2510×(AMW) + 0.8064×(GATS7m) + 0.8258×(GATS4e) + 3.0130×(CID2) - 0.2505×(-CH< [aromatic attach]) - 0.2075×(=CH [aliphatic attach]) - 9.4956**

Table 5. Statistical validation of FDA cluster model fit results for rutin

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.967 (29 out of 30)	1.000 (18 out of 18)	0.917 (11 out of 12)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-4.5197	2.0215
Mp	Mean atomic polarizability (scaled on Carbon atom)	8.3104	3.2103
MATS3m	Moran autocorrelation - lag 3 / weighted by atomic masses	-1.7100	0.5420
-C(=O)- [aromatic attach]	-C(=O)- [aromatic attach] fragment count	-0.4779	0.1622
-C(=O)O- [cyclic]	-C(=O)O- [cyclic] fragment count	-0.5967	0.2186
Intercept	Model intercept	-4.5197	2.0215

***value for 90% confidence interval; *Model equation:* Mutagenicity = 8.3104×(Mp) - 1.7100×(MATS3m) - 0.4779×(-C(=O)- [aromatic attach]) - 0.5967×(-C(=O)O- [cyclic]) - 4.5197**

Table 6. Statistical validation of FDA cluster model fit results for phenolic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.971 (34 out of 35)	0.857 (6 out of 7)	1.000 (28 out of 28)	35

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	0.6370	0.4742
SssNH_acnt	Count of (– NH –) (SssNH_acnt)	0.6064	0.2805
MDEN23	Molecular distance edge between all secondary and tertiary nitrogens	0.5657	0.2961
MATS1m	Moran autocorrelation - lag 1 / weighted by atomic masses	1.3119	0.5425
GATS3p	Geary autocorrelation - lag 3 / weighted by atomic polarizabilities	-0.5142	0.3933
piPC08	Molecular multiple path count of order 08	0.0449	0.0377
ALOGP2	Ghose-Crippen octanol water coefficient squared	-0.0371	0.0276
-CH2- [aromatic attach]	-CH2- [aromatic attach] fragment count	-0.2872	0.2012

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.6064×(SssNH_acnt) + 0.5657×(MDEN23) + 1.3119×(MATS1m) - 0.5142×(GATS3p) + 0.0449×(piPC08) - 0.0371×(ALOGP2) - 0.2872×(-CH2- [aromatic attach]) + 0.6370**

Table 7. Statistical validation of FDA cluster model fit results for epigallocatechin gallate

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.900 (27 out of 30)	1.000 (21 out of 21)	0.667 (6 out of 9)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	0.9000	0.1195
SaaaC_acnt	Count of (aaaC) (SaaaC_acnt)	-0.2250	0.0991
=C [aliphatic attach]	=C [aliphatic attach] fragment count	0.7500	0.3778
-C(=O)- [aromatic attach]	-C(=O)- [aromatic attach] fragment count	-0.9000	0.2926

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.2250×(SaaaC_acnt) + 0.7500×(=C [aliphatic attach]) - 0.9000×(-C(=O)- [aromatic attach]) + 0.9000**

Table 8. Statistical validation of FDA cluster model fit results for coumarin

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.967 (29 out of 30)	0.909 (10 out of 11)	1.000 (19 out of 19)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	2.3702	1.2622
SsNH2_acnt	Count of (– NH2) (SsNH2_acnt)	1.4367	0.4114

SdO_acnt	Count of (= O) (SdO_acnt)	0.2865	0.1865
SssO_acnt	Count of (– O –) (SssO_acnt)	-0.6127	0.2654
Qsv	Average of Qs and Qv	-2.3246	1.6333
GATS4e	Geary autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	-0.6539	0.4283
Hy	hydrophilic factor	-0.3022	0.2617

***value for 90% confidence interval; *Model equation:* Mutagenicity = 1.4367×(SsNH2_acnt) + 0.2865×(SdO_acnt) - 0.6127×(SssO_acnt) - 2.3246×(Qsv) - 0.6539×(GATS4e) - 0.3022×(Hy) + 2.3702**

Table 9. Statistical validation of FDA cluster model fit results for quercetin

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.829 (29 out of 35)	0.913 (21 out of 23)	0.667 (8 out of 12)	35

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	0.8400	0.1313
>C= [aromatic attach]	>C= [aromatic attach] fragment count	-0.6400	0.2456

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.6400×(>C= [aromatic attach]) + 0.8400**

Table 10. Statistical validation of FDA cluster model fit equation for psoralen

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.867 (26 out of 30)	0.833 (15 out of 18)	0.917 (11 out of 12)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-2.9473	2.6841
SsaaC	Sum of (saaC) E-States (SsaaC)	-0.1832	0.1297
icycem	Mean information on the vertex cycle matrix equality	4.4262	2.7724
nN	Number of Nitrogen atoms	0.2018	0.1389
GATS3v	Geary autocorrelation - lag 3 / weighted by atomic van der Waals volumes	-0.6701	0.5176

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.1832×(SsaaC) + 4.4262×(icycem) + 0.2018×(nN) - 0.6701×(GATS3v) - 2.9473**

Table 11. Statistical validation of FDA cluster model fit results for bergapten

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.900 (27 out of 30)	0.947 (18 out of 19)	0.818 (9 out of 11)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	3.5806	0.8893
SsaaC	Sum of (saaC) E-States (SsaaC)	-0.2423	0.1232
MAXDP	Maximal electrotopological positive variation	-0.2486	0.0981

MATS5m	Moran autocorrelation - lag 5 / weighted by atomic masses	0.6274	0.5404
GATS2v	Geary autocorrelation - lag 2 / weighted by atomic van der Waals volumes	-0.9330	0.7510
GATS3p	Geary autocorrelation - lag 3 / weighted by atomic polarizabilities	-0.8863	0.5886

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.2423×(SsaaC) - 0.2486×(MAXDP) + 0.6274×(MATS5m) - 0.9330×(GATS2v) - 0.8863×(GATS3p) + 3.5806**

Table 12. Statistical validation of FDA cluster model fit results for kaempferol

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.833 (25 out of 30)	0.889 (16 out of 18)	0.750 (9 out of 12)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	0.8239	0.1484
ic	Information content	-0.1194	0.0900
>C= [aromatic attach]	>C= [aromatic attach] fragment count	-0.4328	0.2846

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.1194×(ic) - 0.4328×(>C= [aromatic attach]) + 0.8239**

Table 13. Statistical validation of FDA cluster model fit results for zeatin

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.967 (29 out of 30)	1.000 (21 out of 21)	0.889 (8 out of 9)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-27.4710	6.0672
SsssN_acnt	Count of (> N –) (SsssN_acnt)	0.5736	0.3427
nN	Number of Nitrogen atoms	0.1438	0.0807
MATS6m	Moran autocorrelation - lag 6 / weighted by atomic masses	-0.7218	0.6776
CID2	Average Randic Connectivity ID number	13.3854	2.9030
-CH< [aliphatic attach]	-CH< [aliphatic attach] fragment count	0.1071	0.0891
-NH- [aromatic attach]	-NH- [aromatic attach] fragment count	0.1843	0.1778

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.5736×(SsssN_acnt) + 0.1438×(nN) - 0.7218×(MATS6m) + 13.3854×(CID2) + 0.1071×(-CH< [aliphatic attach]) + 0.1843×(-NH- [aromatic attach]) - 27.4710**

Table 14. Statistical validation of FDA cluster model fit results for gallic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.933 (28 out of 30)	0.923 (12 out of 13)	0.941 (16 out of 17)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	3.5421	1.0840
SdssNp	Sum of (= N+ <) E-States (SdssNp)	-1.4262	0.3039
SHother	Sum of (CH or CH2 with -F or -Cl attached) hydrogen E-State values (SHCHnX)	-0.2405	0.1112
GATS3v	Geary autocorrelation - lag 3 / weighted by atomic van der Waals volumes	-1.8747	0.7018
XLOGP2	Wang octanol water partition coefficient squared	-0.0851	0.0651

***value for 90% confidence interval; *Model equation:* Mutagenicity = -1.4262×(SdssNp) - 0.2405×(SHother) - 1.8747×(GATS3v) - 0.0851×(XLOGP2) + 3.5421**

Table 15. Statistical validation of FDA cluster model fit results for ellagic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.940 (47 out of 50)	1.000 (37 out of 37)	0.769 (10 out of 13)	50

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	2.0333	0.9248
SdssC_acnt	Count of (= C <) (SdssC_acnt)	-0.2215	0.1140
nR10	Number of 10-membered rings	0.2824	0.1436
MATS1e	Moran autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities	1.3238	1.0556
MATS5p	Moran autocorrelation - lag 5 / weighted by atomic polarizabilities	0.9161	0.4953
GATS6p	Geary autocorrelation - lag 6 / weighted by atomic polarizabilities	-1.2098	0.9149
XLOGP2	Wang octanol water partition coefficient squared	-0.0439	0.0146
=C [aliphatic attach]	=C [aliphatic attach] fragment count	1.3197	0.4198
-C(=O)- [aromatic attach]	-C(=O)- [aromatic attach] fragment count	-0.6433	0.3247

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.2215×(SdssC_acnt) + 0.2824×(nR10) + 1.3238×(MATS1e) + 0.9161×(MATS5p) - 1.2098×(GATS6p) - 0.0439×(XLOGP2) + 1.3197×(=C [aliphatic attach]) - 0.6433×(-C(=O)- [aromatic attach]) + 2.0333**

Table 16. Statistical validation of FDA cluster model fit results for chlorogenic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.933 (28 out of 30)	0.938 (15 out of 16)	0.929 (13 out of 14)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-2.1907	1.2731
GATS5e	Geary autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities	2.7009	1.3218
-CH2- [aliphatic attach]	-CH2- [aliphatic attach] fragment count	-0.0741	0.0480
-C(=O)- [2 aromatic attach]	-C(=O)- [2 aromatic attach] fragment count	0.3748	0.0948

***value for 90% confidence interval; *Model equation:* Mutagenicity = 2.7009×(GATS5e) - 0.0741×(-CH2- [aliphatic attach]) + 0.3748×(-C(=O)- [2 aromatic attach]) - 2.1907**

Table 17. Statistical validation of FDA cluster model fit results for vanillic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	1.000 (30 out of 30)	1.000 (12 out of 12)	1.000 (18 out of 18)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	6.6733	1.5053
SdssNp_acnt	Count of (= N+ <) (SdssNp_acnt)	0.9518	0.1341
BEHm7	Highest eigenvalue n. 7 of Burden matrix / weighted by atomic masses	0.3586	0.1571
Lop	Lopping centric index	-5.8296	1.3011
-OH [aromatic attach]	-OH [aromatic attach] fragment count	-0.2685	0.0977

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.9518×(SdssNp_acnt) + 0.3586×(BEHm7) - 5.8296×(Lop) - 0.2685×(-OH [aromatic attach]) + 6.6733**

Table 18. Statistical validation of FDA cluster model fit results for ferulic acid

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.933 (28 out of 30)	0.875 (7 out of 8)	0.955 (21 out of 22)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-2.0168	0.6601
SsCH3_acnt	Count of (– CH3) (SsCH3_acnt)	-0.1568	0.1417
ATS8m	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic masses	0.1623	0.0994
GATS7e	Geary autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	0.1681	0.1146
GATS4p	Geary autocorrelation - lag 4 / weighted by atomic polarizabilities	1.7063	0.4749

***value for 90% confidence interval; *Model equation:* Mutagenicity = -0.1568×(SsCH3_acnt) + 0.1623×(ATS8m) + 0.1681×(GATS7e) + 1.7063×(GATS4p) - 2.0168**

Table 19. Statistical validation of FDA cluster model fit results for β-carotene

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.967 (29 out of 30)	1.000 (6 out of 6)	0.958 (23 out of 24)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	2.3601	1.3686
Ms	Mean electrotopological state	0.5582	0.3686
ATS3p	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic polarizabilities	-1.0138	0.3277
ATS7p	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic polarizabilities	0.1636	0.1516

***value for 90% confidence interval; *Model equation:* Mutagenicity = 0.5582×(Ms) - 1.0138×(ATS3p) + 0.1636×(ATS7p) + 2.3601**

Table 20. Statistical validation of FDA cluster model fit results for β-sitosterol

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.886 (31 out of 35)	0.500 (4 out of 8)	1.000 (27 out of 27)	35

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-0.2724	0.2420
MDEN23	Molecular distance edge between all secondary and tertiary nitrogens	14.9624	6.0149
-CH< [aliphatic attach]	-CH< [aliphatic attach] fragment count	0.0728	0.0408
-O- [oxygen attach]	-O- [oxygen attach] fragment count	0.7265	0.3733

***value for 90% confidence interval; *Model equation:* Mutagenicity = 14.9624×(MDEN23) + 0.0728×(-CH< [aliphatic attach]) + 0.7265×(-O- [oxygen attach]) - 0.2724**

Table 21. Statistical validation of FDA cluster model fit results for skimmianine

Prediction statistics				
Endpoint	**Concordance**	**Sensitivity**	**Specificity**	**# chemicals**
Mutagenicity	0.933 (28 out of 30)	0.941 (16 out of 17)	0.923 (12 out of 13)	30

Model coefficients			
Coefficient	**Definition**	**Value**	**Uncertainty***
Intercept	Model intercept	-15.4107	9.6378
BEHe1	Highest eigenvalue n. 1 of Burden matrix / weighted by atomic Sanderson electronegativities	5.8992	1.9450
BEHp2	Highest eigenvalue n. 2 of Burden matrix / weighted by atomic polarizabilities	-2.1994	1.2646
MATS7e	Moran autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	0.3006	0.2941
SRW09	Self-returning walk count of order 9	-0.0002	0.0001
-OH [aromatic attach]	-OH [aromatic attach] fragment count	-0.3624	0.3027

***value for 90% confidence interval; *Model equation:* Mutagenicity = 5.8992×(BEHe1) - 2.1994×(BEHp2) + 0.3006×(MATS7e) - 0.0002×(SRW09) - 0.3624×(-OH [aromatic attach]) - 15.4107**

.DISCUSSION

Biodiversity study of plant species was an established research work to know ecosystem sustainability. Many researchers have been documented medicinal plant diversity in local area, parks, avenues, suburban area, forests etc. (Chantia, 2003; Jain et al., 2005; El-Wahab, 2008; Lal and Singh, 2012; Bhat et al., 2013; Talapatra, 2013; Das et al., 2015). Moreover, diversity of medicinal plant species is a matter of great concern to achieve the traditional knowledge finally leads to discovery of herbal medicine by the presence of bioactive compounds, which has immense potential to health care with special reference to prevent several diseases and majorly mutation and cancer of human beings (Agarwal and Pandey, 2009; Ahmed and Urooj, 2010; Satwinderjeet et al., 2010; Talapatra et al., 2010; Ramila Devi and Manoharan, 2011; Sanjib, 2011; Shivalinge et al., 2011; Barangi et al., 2012; Satish et al., 2013; Sinhababu and Banerjee, 2013; Espanha et al., 2014; Joselin et al., 2014; Shad et al., 2014; Das et al., 2015).
The study of mutagenicity or antimutagenicity in *Salmonella typhimurium* TA97, TA98, TA100 and TA102 test strains were used in the Ames test, which is a biological assay to assess the mutagenic or antimutagenic potential of chemical compounds designed by the American biologist Bruce N. Ames (Maron and Ames, 1983; Purohit and Basu, 2000). However, this experimental study have already well established but some constrains like time consuming screening, chemical expenses, proper laboratory facilities etc. should be required to complete the experiments. There are more than hundreds QSAR models have been established on genotoxicity prediction, among them QSAR modeled Ames mutagenicity T.E.S.T. software (USEPA, 2012) is a potent modeling endpoint for genotoxicity. It is very interesting to note that QSAR modeling by using software can also predict the potent toxic or mutagenic or antimutagenic compounds with the help of physical structures and suitable molecular descriptors functioning in the computer simulation (Hansch and Leo, 1995; Franke and Gruska, 2003; Benigni, 2005; de Melo et al. 2010; USEPA, 2012; Talapatra et al., 2015).

It was previously studied that bioactive compound as epigallocatechin gallate was antimutagenic found in tea (Hour et al., 1999) and leaf extracts of *M. indica* but present result was contradicted for antimutagenicity prediction for active compound of *M. indica*. According to Haslam, (1996) and Labieniec et al., (2003; 2007), some flavonoids are mutagenic and in experimental study the mangiferin may be induced antimutagenic (Rodeiro et al., 2006) alongwith other compounds (Hernandez et al., 2007). In Table 2, the bioactive compound quercetin is mutagenic in purified form to *Salmonella typhimurium* (Bieldanes and Chang, 1977; Stoewsand et al., 1984) and also previous study on QSAR modeling this compound was also mutagenic when studied in the absence of the mutagen (Edenharder and Tang, 1997; de Melo et al., 2010) while zeatin polyphenol and skimmianine alkaloid were also reported mutagenic by other researchers (Basha et al., 2013; Hafele and Schimmer, 1988) and the prediction data was also observed mutagenic that has close similarities with present results. The ellagic acid was reported antimutagenic (Dixit and Gold, 1986; Teel, 1986) but present result was showed mutagenic as individual compound and higher dose of this compound caused genotoxicity in freshwater mussels (Labieniec et al., (2007). However, it showed antimutagenic in experimental study that might be of cumulative effect with other compounds present in plant parts or may act upon particular mutagen. Moreover, phytochemicals viz. catechin, flavonol, rutin, phenolic acid, lupeol, coumarin, psoralen, bergapten, kaempferol, friedelin, gallic acid, chlorogenic acid, vanillic acid, ferulic acid and β-carotene and sterols viz. β-sitosterol were predicted antimutagenic compounds. This present data have close similarities with experimental Ames mutagenicity assay by other researchers (de Melo et al., 2010; Rinaldo et al., 2010; Satish et al., 2013; Espanha et al., 2014) except bergapten, coumarin and β-carotene were reported mutagenic during experimental study (Judson et al., 2005) and also in software database, which has contradicted prediction in the present results.

According to Contrera et al. (2005), the binary (active/inactive) mutagenicity endpoints, the prediction accuracy is evaluated in terms of the fraction of chemicals for accurate prediction. Generally, the prediction accuracy is evaluated in terms of three different statistical parameters viz. concordance, sensitivity, and specificity. Concordance is the fraction of all similar chemicals that are predicted correctly it means experimentally active compounds will be predicted active and experimentally inactive compounds will not be predicted active). Sensitivity is the fraction of experimentally active compounds will be predicted active. Specificity is the fraction of experimentally inactive compounds will not be predicted active (USEPA, 2012). The FDA cluster model for mutagenicity positive or negative prediction through T.E.S.T. software, the average concordance (accuracy) values for studied phytochemicals such as catechin (86.7%), flavonol (94.3%), rutin (96.7%), phenolic acid (97.1%), epigallocatechin gallate (90.0%), coumarin (96.7%), quercetin (82.9%), psoralen (86.7%), bergapten (90.0%), kaempferol (83.3%), zeatin (96.7%), gallic acid (93.3%), ellagic acid (94.0%), chlorogenic acid (93.3%), vanillic acid (100.0%), ferulic acid (93.3%), β-carotene (96.7%), β-sitosterol (88.6%) and skimmianine (93.3%) were observed (Table 3 – 21). The present study was based on the prediction data available after calculating with CAS no. of particular compound in the T.E.S.T. software and the data expressed as per obtaing predictive results. According to Votano et al. (2004), the compound's biological activity can be determined by using QSAR model to predict genotoxicity correlates the chemical structure, given in terms of continuous or binary molecular descriptors. Different types of descriptors have been used in predictive models for Ames bacterial mutagenicity test by many researchers viz. chemical substructures studied by Klopman et al. (1984; 1990), topological parameters in QSAR by Basak et al. (2001), TOPKAT software prediction (Accelrys Inc., 2003), logP and electronic parameters studied by King et al. (1996) and combinations of different classes of descriptors viz. geometric, electronic, polar surface area and topological studied by Mattioni et al. (2003). The T.E.S.T. predictions for Ames mutagenicity positive and negative values for *Salmonella typhimurium*, the suitable molecular descriptors include the classes of descriptors viz. Constitutional descriptors, Chi Connectivity Indices, Kappa Shape Indices, Electrotopological State Indices, Fragments for each atom, 2D Molecular properties (such as the octanol-water partition coefficient), Information Indices, Burden eigenvalue descriptors, Topological descriptors, Walk and Path counts, 2D Autocorrelation Descriptors, Molecular Properties and Molecular Distance Edge Descriptors (USEPA, 2012).

CONCLUSION

It was concluded that from the above results T.E.S.T. software was predicted so far well in relation to predictive Ames mutagenicity positive and negative assessment for phytochemicals present in studied tree species with concordance (accuracy) values. The present work was based on the prediction data available after calculating with CAS no. entered for particular compound in the T.E.S.T. software and the results were expressed as per as per obtaing predictive data (USEPA, 2012). It is important to note that the studied tree species diversity should be required to maintain and conserve for healthcare management against several mutagens especially to prevent mutation and cancer. Moreover, this present software unable to predict few phytochemicals due to unavailability of CAS no. in the database, which was reported as not found. It was also reported two bioactive compounds viz. lupeol and friedelin did not prescribe cluster FDA model fit results and equation, which is still unknown. This is also suggested, mutagenicity study can be relevant with other QSAR modeling softwares to compare predicted data.

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