CHAPTER

Chemistry of plant extracts

3

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3.1 Introduction

Plant extracts have been used traditionally to cure and prevent diseases throughout the history. Plant extracts are used as preservatives because of their strong antimicrobial and antioxidant activities. The efficacy of plant extracts lies in chemical substances possessed by them, and these compounds are classified as terpenoids, alkaloids, phenolic compounds, glucosinolates, and various organic acids. Plant extract or pure compounds obtained from various plants offer opportunities for food preservation because of their chemical diversity. For centuries, many plant products have been used to improve the sensory characteristics and extend the shelf life of many foods. Plant extracts extend the storage life of foods by controlling the growth of spoilage and pathogenic bacteria and enhance the quality of foods by inhibiting the oxidative rancidity.

The activity of plant extracts is determined by its chemical properties, the solubility being most important for food application, and its pH being the other important factors (Stratford & Eklund, 2003). Active ingredients in plant extracts differ due to many factors such as parts of plant utilized (roots, stems, leaves, bark, flowers, fruits, and seeds), stage of their maturity, genotype, climatic factors, soil factors, cultivation practices, the time of harvesting, postharvest operations, pretreatments before extraction, and the extraction methods. Plant extracts are widely used in the food industry, and this chapter summarizes the extraction of phytochemicals, their chemical composition, and relationship of various chemical structures in plant extracts with biological activities exerted by them for further widening the application of plant extracts in natural preservation.

3.2 Extraction procedures and chemical composition of plant extracts

The procedure adopted for the extraction of compounds from plants determines the quality and quantity of plant extracts. Various extraction methods followed include solvent extraction (water, ethanol, methanol, and other solvents) (Pinelo, Rubilar, Jerez, Sineiro, & Núñez, 2005; Ye, Liang, Li, & Zhao, 2015), pressurized-liquid extraction (Luthria, 2008), supercritical-fluid extraction (Inczedy, Lengyel, & Ure, 1998; Temelli & Güçlü-Üstündağ, 2005), and various assisted extraction techniques, such as the microwave-assisted extraction (Alupului, Calinescu, & Lavric, 2012), ultrasound assisted extraction (Herrera & De Castro, 2005), and enzyme assisted extraction (Rosenthal,

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Pyle, & Niranjan, 1996). Before the extraction of any bioactive compound, it is also important to consider the developmental stage and plant part accumulating the bioactive compound. A distribution of various chemical classes of bioactive compounds present in plants is presented in Table 3.1. The plant extracts can be quantified for the presence of active compounds by various

Table 3.1 Distribution of various chemical classes of bioactive compounds in plants.

Chemical class of bioactive compound	Distribution of bioactive compounds in plants (developmental stage/tissue/plant part)	References
Monoterpenes Sesquiterpenes	Development and growth phase; aerial parts of plants	Aharoni et al. (2003)
Glucosinolates	High content in seeds, siliques, and young leaves; moderate content in roots, stems, and leaves; and low content in senescing leaves	Brown, Tokuhisa, Reichelt, and Gershenzon (2003)
Anthocyanins	Vegetative tissue and embryo	Lepiniec et al. (2006)
Proanthocyanidins	Endothelium of developing seed coats	
Flavonols	Vegetative and reproductive tissues	
Flavan-4-ol 3-deoxyflavonoids apiferol & luteoferol	Pericarp	
Isoflavones	Embryo and seed coat	Halkier and Gershenzon (2006)
Benzylisoquinoline-derived alkaloids	Accumulates in specialized cell present in vascular tissues known as laticifers	Bird, Franceschi, and Facchini (2003), Weid, Ziegler, and Kutchan (2004)
Myrosinase and glucosinolates	Distinct subcellular compartments	Grubb and Abel (2006)
Limonene	*Pinus ponderosa:* bark	Harborne (1986, 1989, 1993, 1997)
Pulegone and carvone	*Satureja douglasii*: leaf	
Lactucin 8-deoxylactucin	*Cichorium intybus*: leaf	
Caryophyllene epoxide	*Melampodium divaricatum:* leaf	
Zingiberene	*Lycopersicon hirsutum:* leaf trichome	
Germacrone	*Ledum groenlandicum*: leaf	
Kaurenoic Trachylobanoic acids	Floret of sunflower (*Helianthus annuus)*	
Camphor	White spruce: leaf	
Alkaloids Cyanogens Monoterpenoids Diterpenoids	Seeds	Harborne and Baxter (1996)
Tannins	Fruits of persimmon (*Diospyros kaki)*	Harborne (1999)
Saponins	Holly (*Ilex opaca*): juvenile leaves Leek (*Allium porrum)*:flowers	
Sesquiterpenes: (*E*)-β-farnesene, β-humulene, and (γ)-muurolene	*Chrysothamnus nauseasus*: leaves	

chromatographic techniques. Plant extracts are available in various forms such as spray-dried powders, pure active ingredients, and encapsulated forms. A general flow diagram for extraction, quantification, and utility of plant extracts is presented in Fig. 3.1.

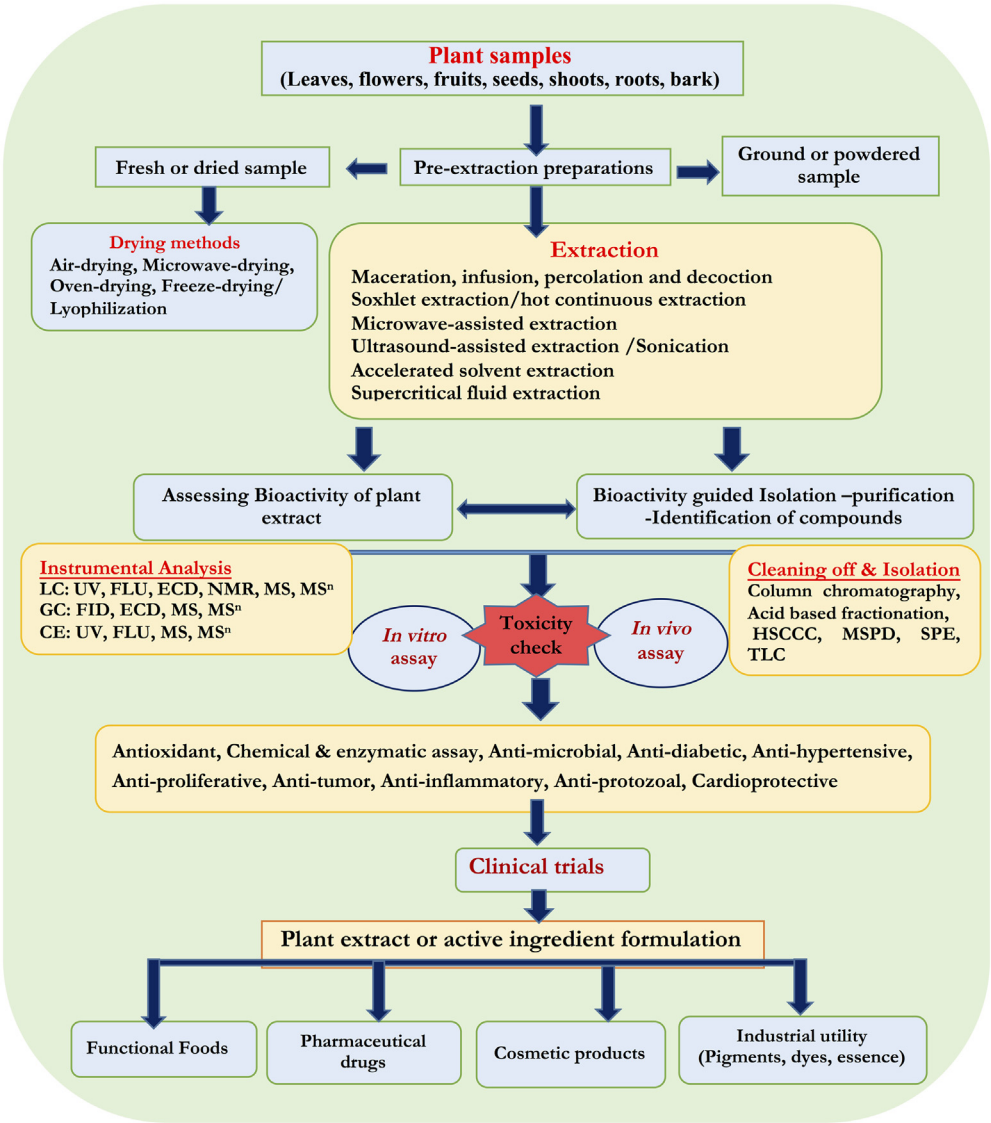


FIGURE 3.1

General scheme of extraction, identification, and utilization of plant extracts.

Various fruits, vegetables, herbs, and spices are used to extract the natural bioactive compounds (Dimitrios, 2006). Several plant extracts or molecules from plants have been commercialized, like moso bamboo (Takeguard) of Takex Labo (Japan) or blend of several natural extracts including green tea (Biovia YM10) by Danisco DuPont, rosemary extract by Naturex's, rosemary extract (Oxikan) by Kancor, and rosemary extract (ExtenFo) by Arjuna Chemicals, India. Members of Punicaceae, Juglandaceae, Rosaceae, Grossulariaceae, Asteraceae, Ericaceae, Empetraceae, and Zingiberaceae families were identified as the main source of plant bioactive compounds (Halvorsen et al., 2002).

3.3 Classification of bioactive compounds in plant extracts

Bioactives in plant extracts are mainly classified as terpenoids, phenolic compounds, glucoinolates, and few miscellaneous compounds. The classification of bioactive compounds based on their chemical structure is discussed in this section, and chemical structures of a few bioactive compounds reported in plant extracts are presented in Fig. 3.2.–3.4.

3.3.1 Terpenoids

Terpenes refer to isoprene polymers and their derivatives with the general formula of (C_5H_8) n, which are most abundantly found in plants and meager in animals. Majority of terpenes form several oxygenated derivatives such as alcohols, aldehydes, ketones, carboxylic acids, esters and glycosides, along with few nitrogen-containing and sulfur-containing derivatives. Terpenoids are hydrocarbons synthesized from isoprene subunits through reactions such as condensation and cyclization, as well they are hydrophobic in nature (Ruchika & Pandey, 2019). Terpenes are categorized depending on their isoprene units, as hemiterpene, monoterpene, sesquiterpene, diterpene, sesterpene, triterpene, tetraterpene and polyterpene (Table 3.2).

Terpenoids compounds have significant role in plants, being a part of important hormones such as gibberellin, abscisic acid and insect juvenile hormone, photosynthetic pigments such as carotenoids and chlorophyll; prominent molecule plastoquinone in photosynthesis and quinone in respiration chain; sterols being the component of the biological membrane. Monoterpene and sesquiterpene can be seen as major component of volatile oil, diterpene in resin; triterpenoid in plant saponins and resins, tetraterpene in some fat-soluble pigments. Few of the bioactivities of terpenoids include roundworm expelling effect by ascaridole and santonin; antimalarial activity by artemisinin, while antibacterial by andrographolidume (Jan & Abbas, 2018; Ruchika & Pandey, 2019).

Carotenoids, the major terpenoids distributed widely in plants, are responsible for different hues and are commonly occurring natural pigments (Namitha & Negi, 2010). Most carotenoids are derived from a 40-carbon structure consisting of eight isoprene units, which includes a system of conjugated double bonds. Carotenoids are classified as carotenes (just carbon and hydrogen atoms) and oxocarotenoids or xanthophylls (minimum one oxygen atom along with carbon and hydrogen). The nature of the specific end groups in carotenoids influences their polarity, and therefore individual carotenoids interact with biological membranes differently (Britton, 1995). Carotenoids

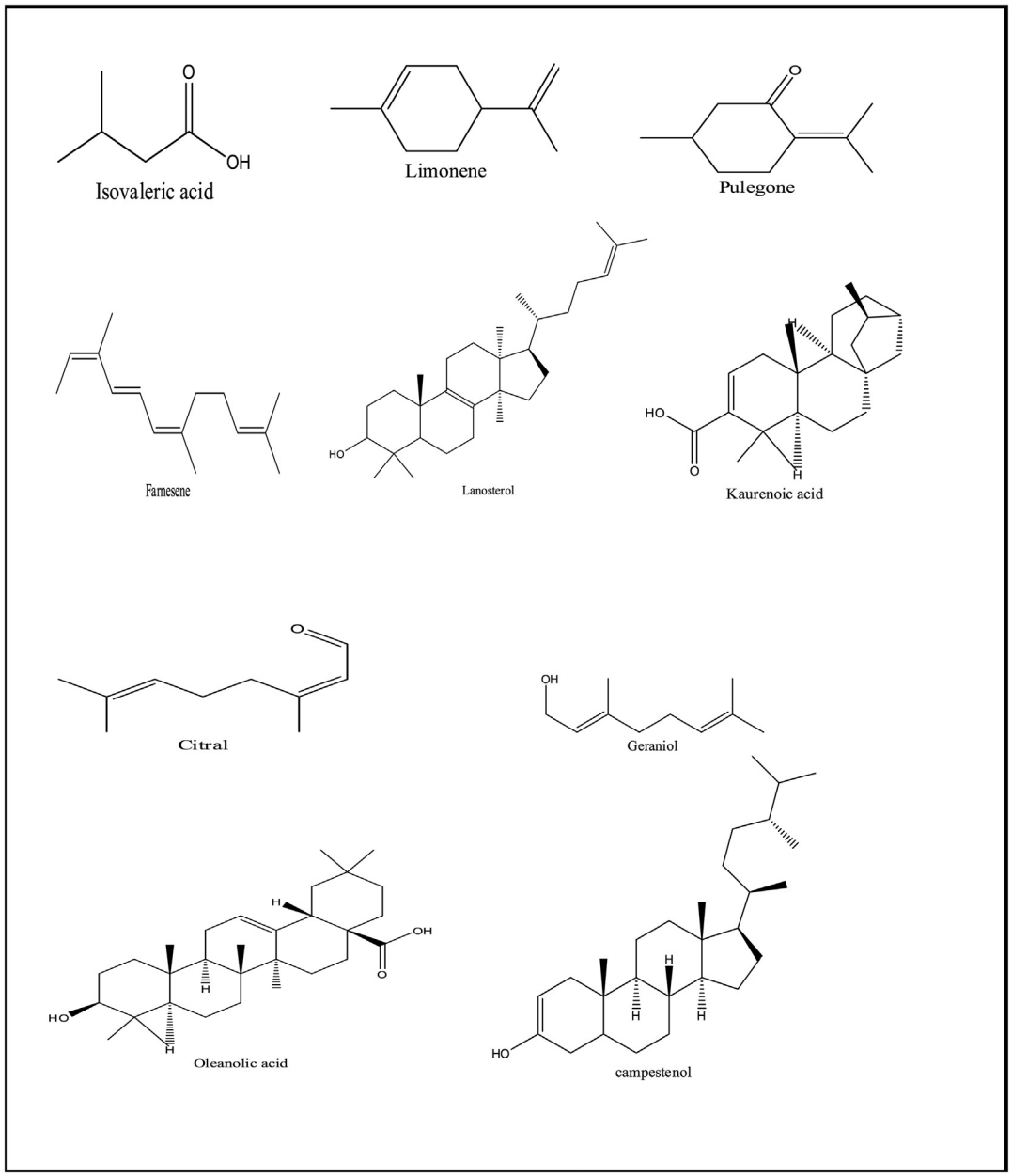
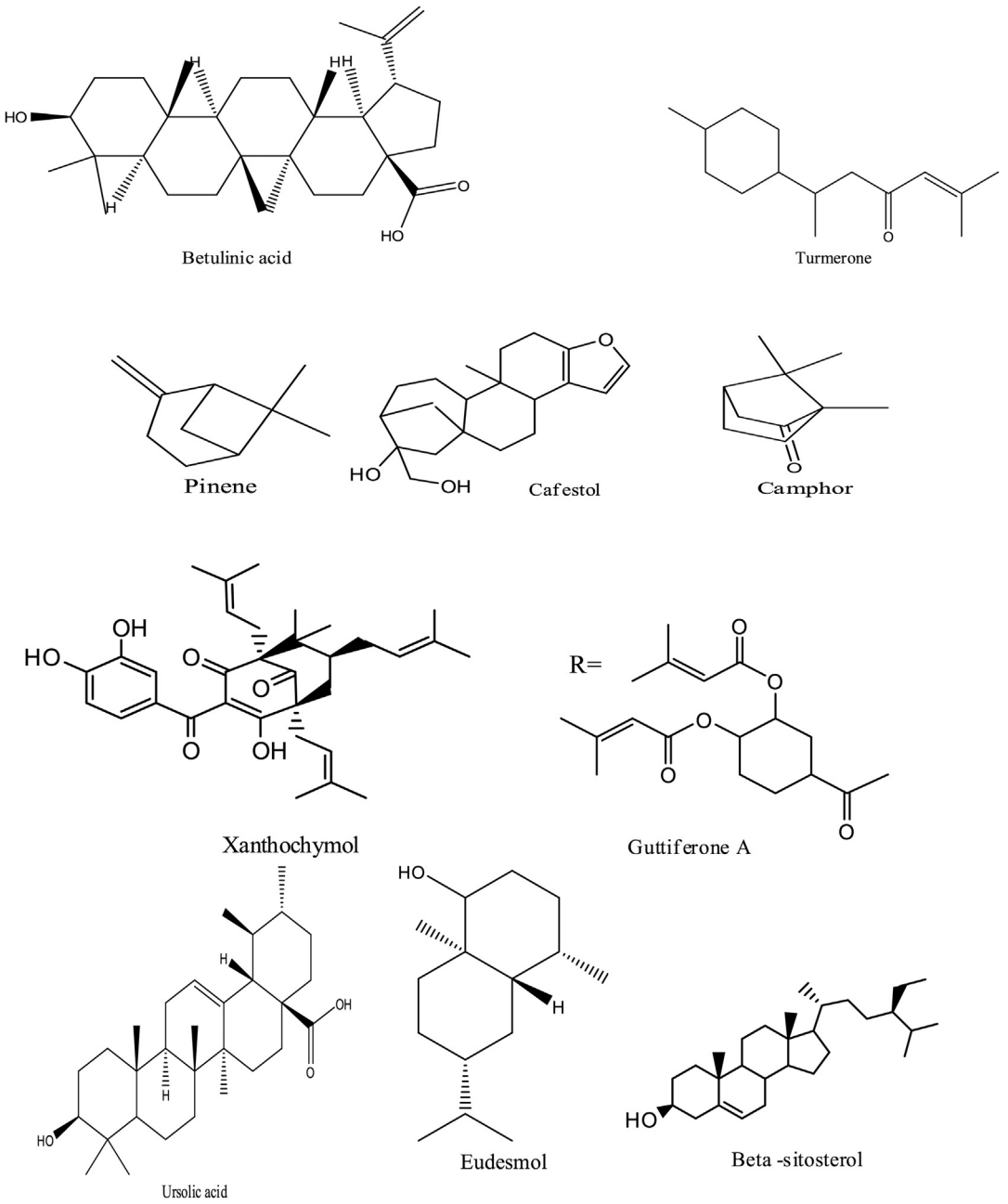


FIGURE 3.2

Chemical structures of terpenoids.



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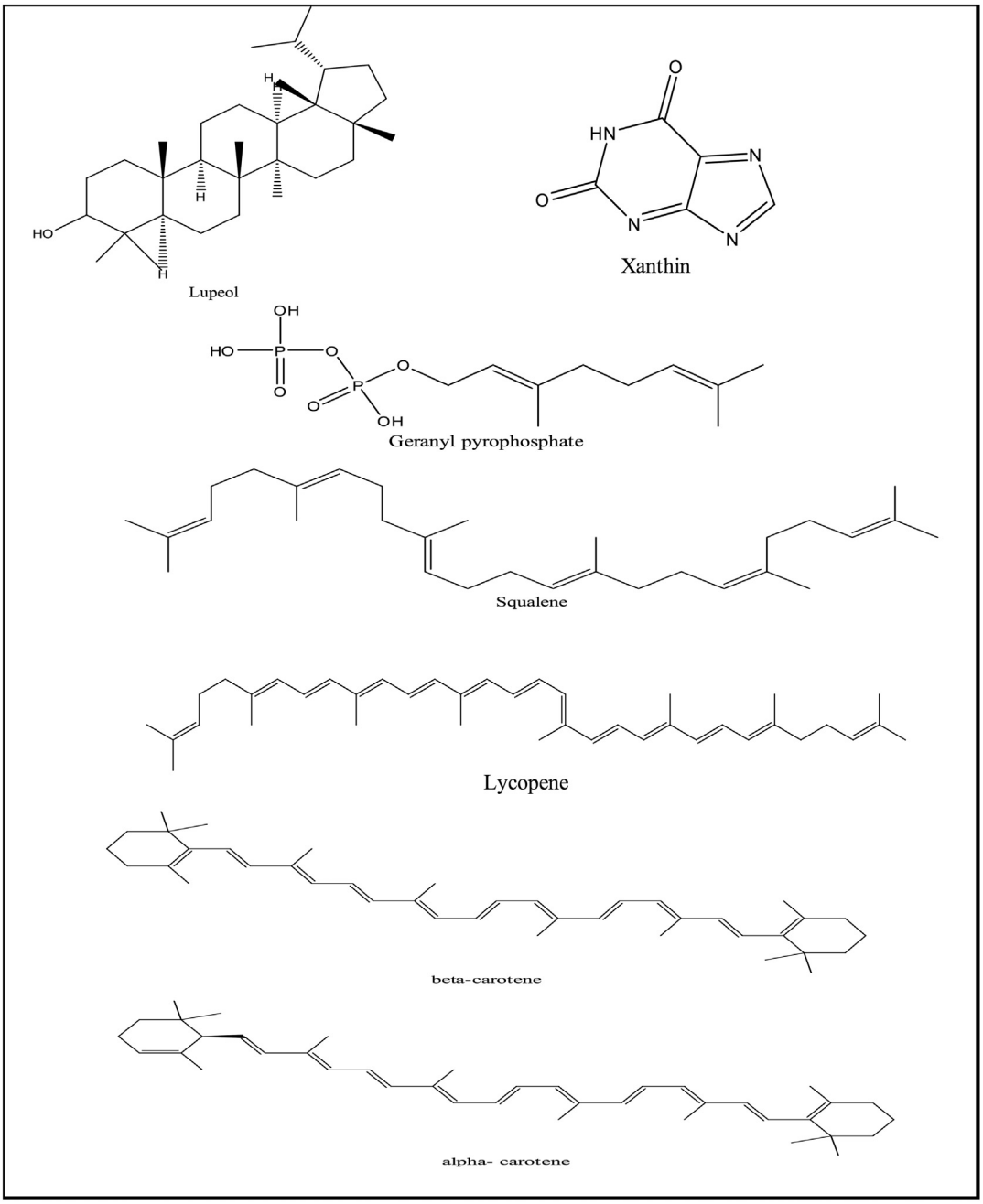

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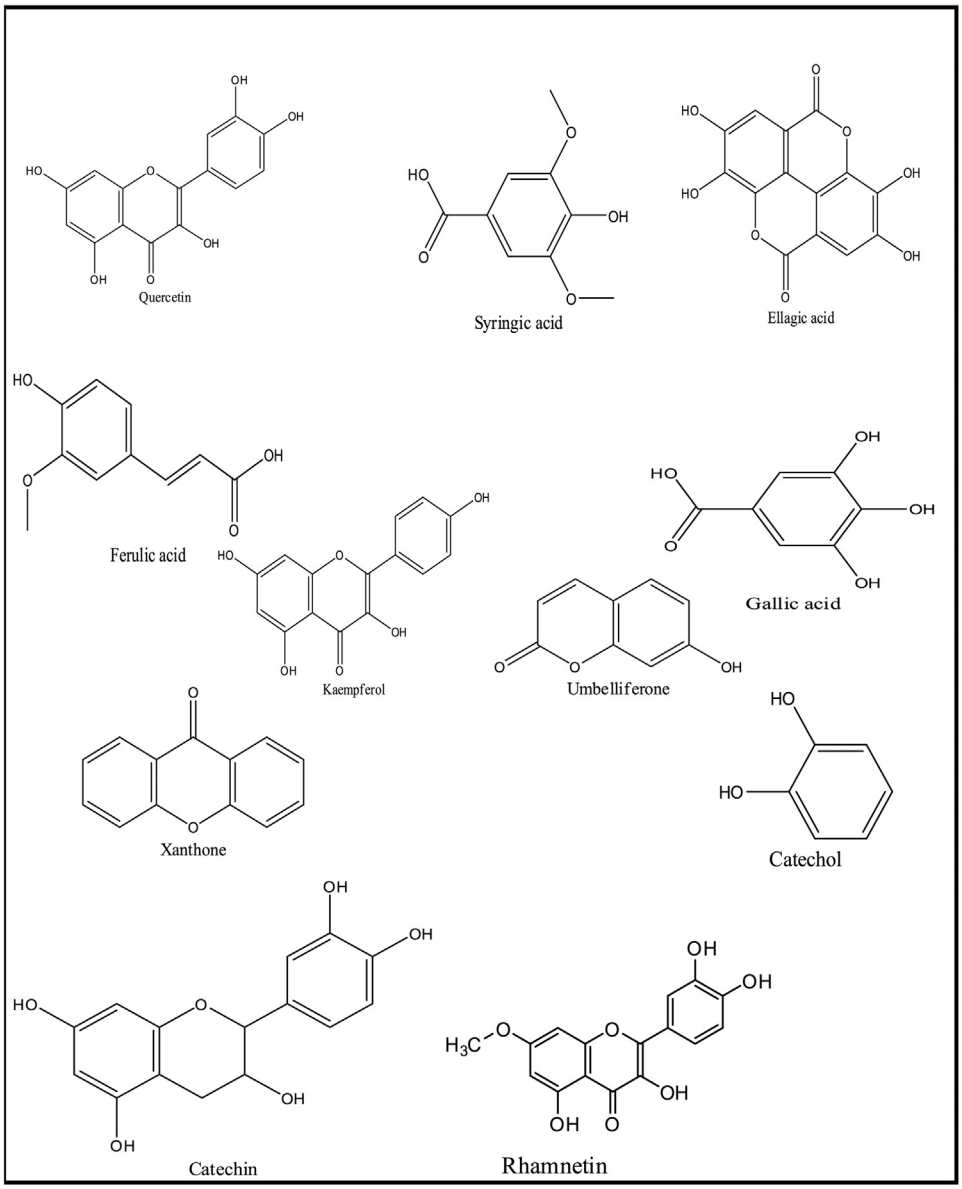
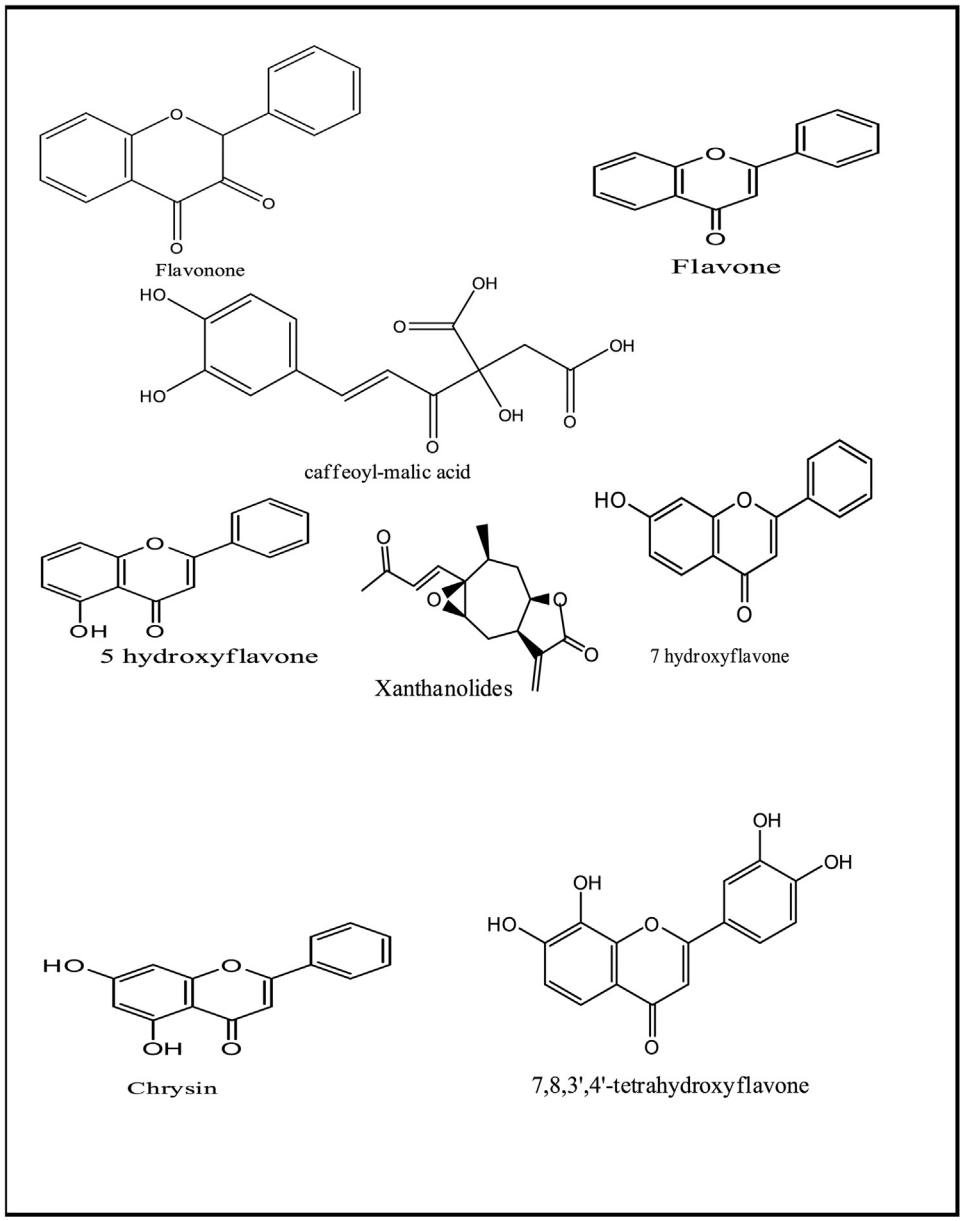


FIGURE 3.3

Chemical structures of phenolic compounds.



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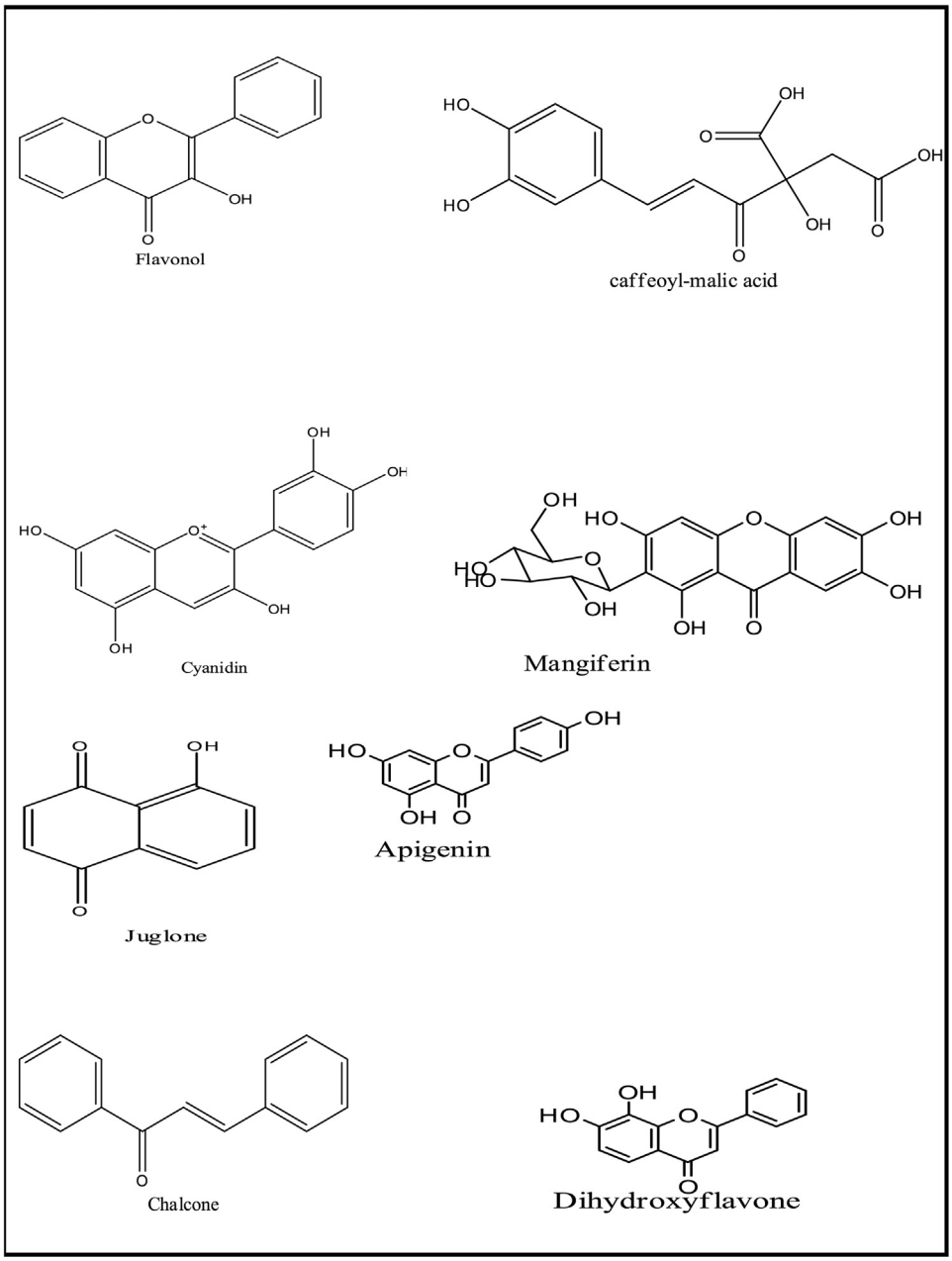

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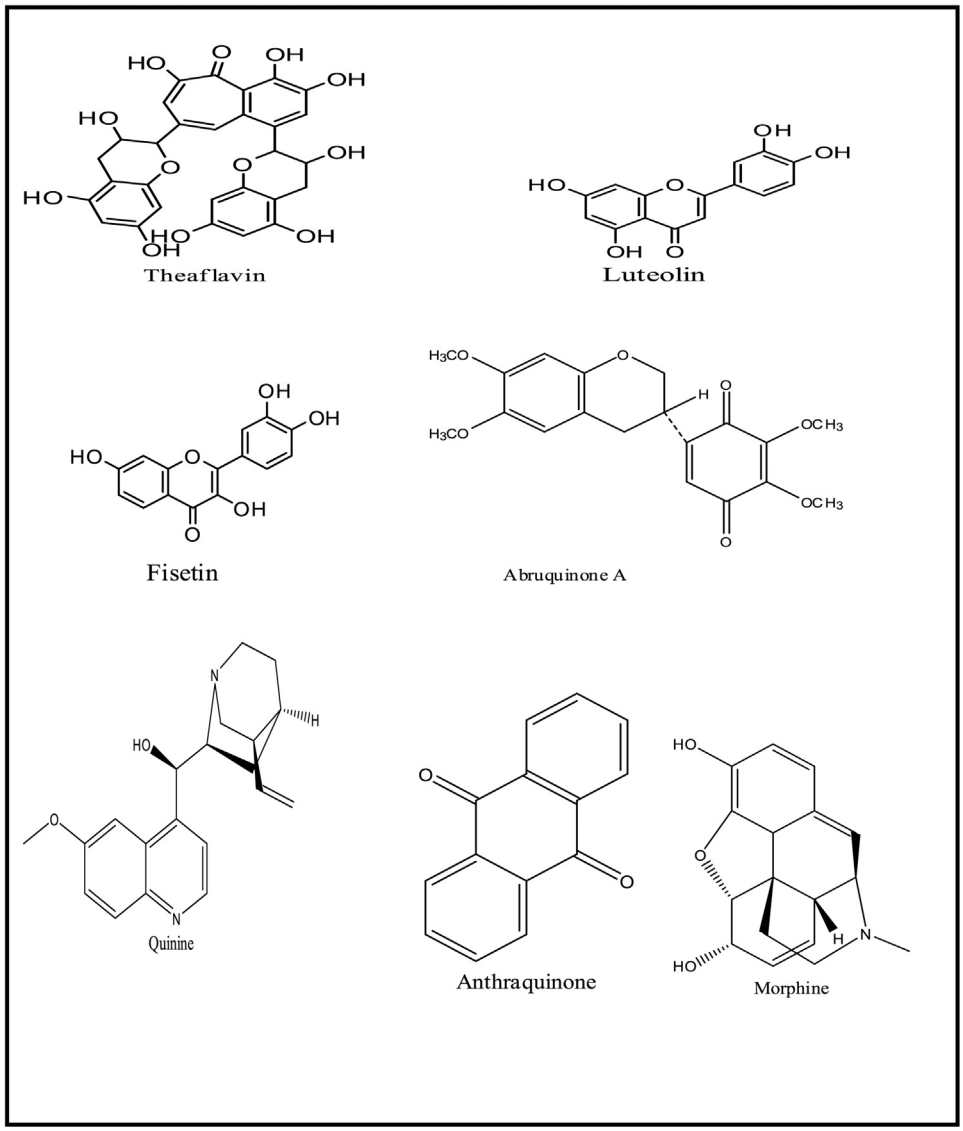

FIGURE 3.3

(Continued)

generally get isomerized and form a mixture of mono- and poly-cis-isomers in addition to the natural all-trans form. Being lipophilic, carotenoids accumulate in lipophilic parts of cells, which influences their absorption, transport and excretion in the organism (Stahl, Schwarz, & Sies, 1993).

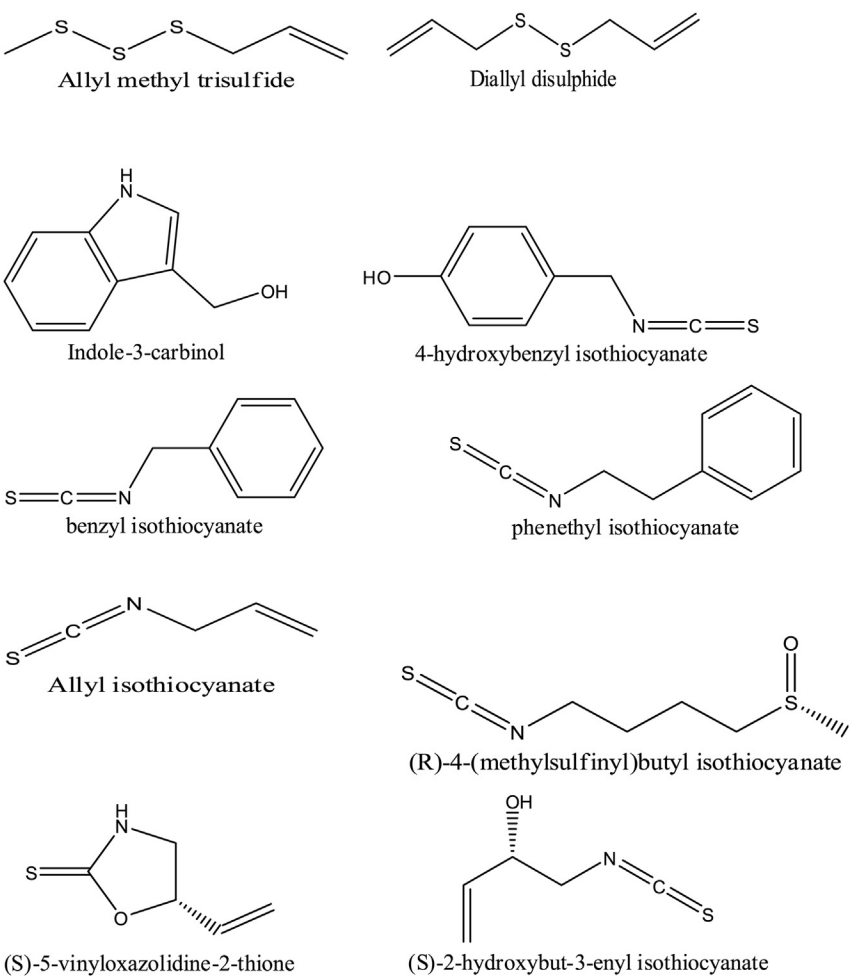

FIGURE 3.4

Chemical structures of glucosinolates.

Carotenoids have excellent antioxidant activity (Sies & Stahl, 1995). Carotenoids are the most potent quenchers of singlet oxygen such as hydrogen peroxide, singlet oxygen, nitrogen oxides, super oxide anion, and other reactive oxygen species (ROS) (Boileau, Moore, & Erdman, 1999; Paiva & Russell, 1999). Carotenoids can deactivate the excited sensitizer molecules involved in the generation of radicals and singlet oxygen (Truscott, 1990; Young & Lowe, 2001). Alternative mechanisms of antioxidant activity of carotenoids include chain-breaking antioxidant to terminate lipid oxidation by β-carotene, and decrease in the release of lactate dehydrogenase to protect cells from lipid peroxidation and membrane damage by β-carotene and lutein (Martin, Failla, & Smith, 1996).

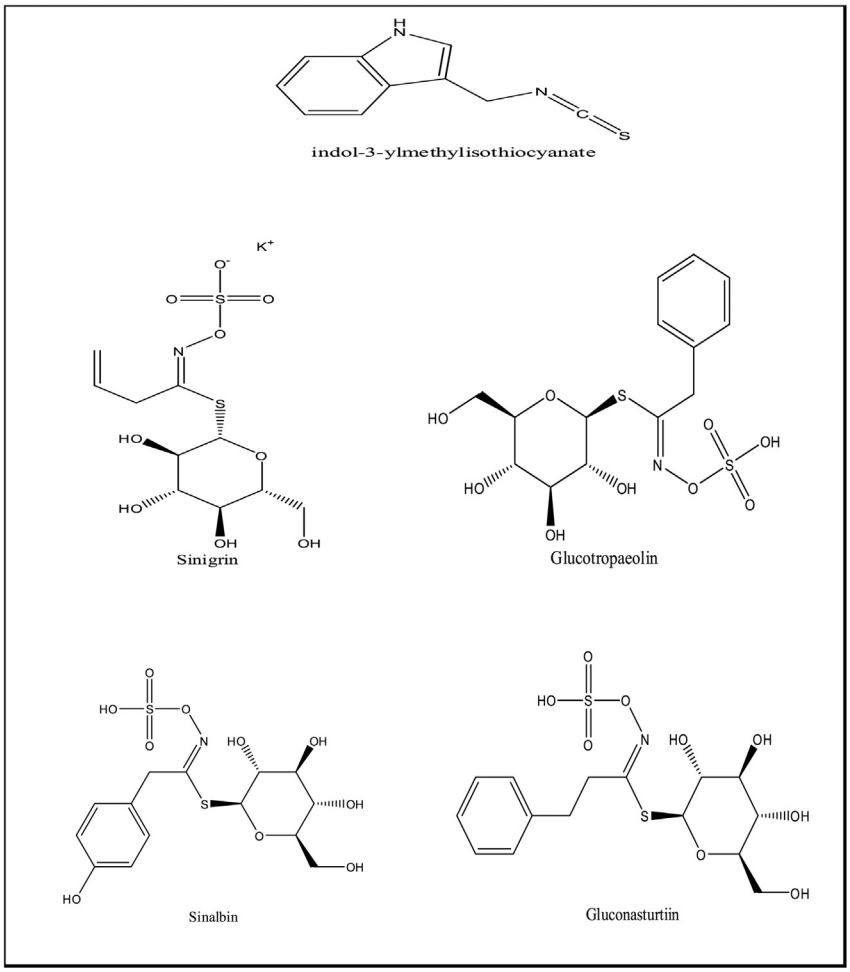

FIGURE 3.4

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3.3.2 Phenolic compounds

Polyphenol is derived primarily from the shikimate-derived phenylpropanoid and/or the polyketide pathway(s), containing more than one phenolic ring. Phenolic compounds are abundantly found in plants and plant derived foods (Rashmi & Negi, 2020a) exhibiting vast variations in their structure, comprising from simple molecules (gallic acid, caffeic acid) to polyphenols (stilbenes, flavonoids, and polymers). Based on the chemical structure, they are grouped into two major groups: flavonoids (flavonols, flavones, flavanols, flavanones, anthocyanidins, isoflavonoids) and nonflavonoids (phenolic acids, stilbenes, coumarins, tannins). The chemical structures of flavonoid show a basic

Table 3.2 Classification of terpenoids.

Class	Structural frame work	Individual compounds
Hemiterpenes	Single isoprene unit	Isovaleric acid Prenol Pulegone
Monoterpenes	C_{10} Two isoprene units	Geraniol Limonene Perillyl alcohol Geranyl pyrophosphate Eucalyptol Citral Camphor Pinene Guttiferone Xanthochymol
Sesquiterpenes	C_{15} Three isoprene units	Artemisinin Bisabolol Fernesol Eudesmol (*E*)-β-farnesene β-humulene (γ)-muurolene Lactone parthenolide
Diterpenes	C_{20} Four isoprene units	Cafestol Cembrene Taxadiene Gibberellins Taxol Kaurenoic acid
Sesterterpenoids	C_{25} Five isoprene units	(2Z,6Z,10E,14E)-Geranylfarnesol C25 analog of transphytol Leucosceptrine Leucosesterterpenone Leucosesterlactone Salvimirzacolide Trinorsesterterpene glycoside Xanthanolides Xanthane
Triterpenoid	C_{30} Six isoprene units	Saponins, Oleanolic acid Ursolic acid Betulinic acid Moronic acid Lanosterol Squalene Azadirachtin b-Amyrin Luperol

Table 3.2 *(Continued)*

Class	Structural frame work	Individual compounds
Sterols	C_{27-30} Six isoprene units	Campesterol Beta Sitosterol Gamma sitosterol Stigmasterol Cholesterol Tocopherols (vitamin E)
Tetraterpenoids/ Carotenoids	C_{40} Eight isoprene units	***Carotenes:*** Orange pigments α-Carotene β- Carotene γ-Carotene δ-Carotene ε-carotene Lycopene ***Xanthophylls:*** yellow pigments Canthaxanthin Cryptoxanthin Zeaxanthin Astaxanthin Lutein Rubixanthin
Polyterpenoids	> C40 More than 8 isoprene units	Rubber

skeleton of diphenyl propane, the two benzene rings (rings A and B) linked with three carbon chains form a pyran ring with benzene ring A. Phenolic compounds are also classified based on number of carbon atoms and carbon skeleton (Table 3.3).

3.3.2.1 Flavonoids and their derivatives

Flavonoids and their derivatives constitute a major class of phytochemicals (Table 3.4). Flavonoids are found in several plants as they impart various color shades to them. They are synthesized from aromatic amino acids by phenylpropanoid pathway. Different classes of flavonoids have same basic structure of benzopyrano moiety and an aromatic ring, existing as glycones or aglycones (Ruchika & Pandey, 2019). Flavonoids are known for their high biological activity such as antimicrobial, antioxidant, anti-carcinogenic and immune enhancing properties.

3.3.2.2 Isoflavonoids

Isoflavonoids class comprises isoflavones, isoflavanones, isoflavans, rotenoids, and pterocarpans, and they are also known as soy flavonoids as they are abundantly present in them. Isoflavonoids exhibit several functional properties such as antioxidant, antimutagenic, anti-carcinogenic, and anti-proliferative (Miadokova, 2009). Isoflavonoids are known as dietary antioxidants, and they protect against free radical damage (Yoon & Park, 2014). The consumption of isoflavonoids is reported to reduce osteoporosis and suppress post-menopausal symptoms (Chen, Ko, & Chen, 2019).

Table 3.3 Classification of phenolic compounds.

No of carbon	Carbon skeleton	Class	Examples
6	C_6	Simple phenol	Catechol
7	C_6-C_1	Hydroxy benzoate	Phenolic acids: gallic, syringic, hydroxy-benzoic acids
9	C_6-C_3	1. Hydroxycinnamate 2. Coumarins	Caffeic, p-coumaric, ferulic, isoferulic scopolatin, aesculetin, umbelliferone
10	C_6-C_4	Napthoquinones	Juglone
13	$C_6-C_1-C_6$	Xanthones	Mangiferin, mangostein
14	$C_6-C_2-C_6$	Stilbenes	Resveratrol
15	$C_6-C_3-C_6$	Flavonoids	Classes of flavonones, anthocyanin
18	$(C_6-C_3)_2$	Lignans	Secosiolariciresinol, matatresinol
30	$(C_6-C_3-C_6)_2$	Biflavonoids	Amentoflavones
N	$(C_6-C_3)_n$	Lignins	Guaiacyl lignins
N	$(C_6-C_3)_n$-Glu	Hydrolysable tannins	Gallotannins, elagitannins, and chebulagic acid
N	$(C_6-C_3-C_6)_n$	Condensed tannins	Proanthocyanidins

3.3.2.3 Lignans

Phenylpropane units are linked by the central carbon (C8) of their propyl side chains in lignans. Lignans differs significantly in the chemical structure of their basic carbon frameworks, oxidation levels, and aromatic substitution patterns (Umezawa, Yamamura, Ono, Shiraishi, & Ragamustari, 2019). Lignans has a class of 2 or 3 molecules of benzene in different forms of polymerization present in both angiosperms and gymnosperms. Plant lignans are polyphenols derivative which are digested by intestinal bacteria to produce mammalian lignans (enerodiol and enterolactone). Lignans are referred as phytoestrogens as they exhibit estrogen agonist and antagonist properties (Pathak et al., 2018; Wcislo & Szarlej-Wcislo, 2014).

3.3.2.4 Tannins

Tannins are high molecular weight compounds (upto 30,000 dalton), which are formed by the polymerization of various flavonoids, and they show typical phenolic reactions with the ability to precipitate proteins, alkaloids, and polysaccharides. Earlier tannins were considered nutritionally undesirable, but lately they have been shown to possess high antioxidant, antimicrobial and anticancer properties. Tannins are classified as hydrolysable and non-hydrolysable tannins based on their acid/ alkali degradation. Hydrolysable tannins are Gallotannins (Glucose polyesters of gallic acid: digalloyl glucose, 1,3,6-trigalloyl glucose, tannic acid, coumarin); Ellagitannins- Glucose polyesters of hexa hydroxy diphenic acid (forms ellagic acid on hydrolysis: punicalagins, castalagins, vescalagins, punicalins, roburin As, terflavin Bs); Taragallotannins- Gallic acid and quinic acid; and caffetannins—caffeic acid and quinic acid. The Non-hydrolysable (condensed) tannins include polymer of flavan-3-ols (proanthocyanidins), polymer of flavan-3,4-diols (leucoanthocyanidins) or mixture of both (flavolans). Further, tannin like compounds formed by oxidation reaction catalyzed by PPO are also reported, and theaflavin, theasinensin, thearubigin, and theacitrin A are present in tea,

Table 3.4 Major flavonoid, isoflavonoid, and alkaloids in plant extracts.

Components	Structural frame work	Individual compounds	References
Flavonoids	C6−C3−C6; Two C6 units at Ring A and Ring B		
Flavan-3-ols/ Flavanols	Hydroxylation and variation in chromane ring (Ring C), Ring B attached to C2 position of Ring C; Flavanol—C2 and C3: double bond absent; Ring C: C4 carbonyl absent	Catechin, epicatechin gallate, epigallocatechin, epigallocatechin gallate, proanthocyanidins, theaflavins, thearubigins, fisetin	Prior, Lazarus, Cao, Muccitelli, and Hammerstone (2001), Tsao (2010)
Anthocyanins		Cyanidin, delphinidin, pelargonidin	Anderson and Jordheim (2006)
Flavanones		Prenylated flavanones, furanoflavanones, pyranoflavanones, benzylated flavanones	Tsao (2010)
Flavonols		Quercetin, kaempferol, rhamnetin	Tsao and McCallum (2009), Valant-Vetschera and Wallenweber (2006), Williams (2006)
Neoflavonoids	Ring B linked to ring C at C4 position	Dalbergin	Garazd, Garazd, and Khilya (2003)
Chalcones	Lack heterocyclic ring C	Phloretin and its glucoside phloridzin (phloretin 2′-0-β-glucopyranoside), chalconaringenin	Tsao (2010)
Flavanonol	15 carbon structure, Ring A and B: 2 phenyl rings Ring C: heterocyclic ring	Taxifolin (dihydroquercetin), aromadedrin (dihydrokaempferol), engeletin (dihydrokaempferol-3-rhamnoside)	Grayer and Veitch (2006), Kawaii, Tomono, Katase, Ogawa, and Yano (1999)
Proanthocyanidins	A-type structure: monomers attached by C2−*O*−C7 or C2−*O*−C5 bond, B−type structure: C4−C6 or C4−C8	Procyanidins, prodelphinidins, propelargonidins	Mateos-Martín, Fuguet, Quero, Pérez-Jiménez, and Torres (2012), Souquet, Cheynier, Brossaud, and Moutounet (1996), Tsao (2010)
Polyphenolic Amides	N-containing functional substituents	Capsaicinoids, avenanthramides	Bratt et al. (2003), Davis, Markey, Busch, and Busch (2007)
Isoflavonoids			
Isoflavones	Ring B connected to C3 position of Ring C	Daidzein, formononetin, genistein, biochanin A, glycetein	Mazur, Duke, Wahala, Rasku, and Adlercreutz (1998), Wang and Murphy (1994)

(*Continued*)

Table 3.4 ***(Continued)***

Components	Structural frame work	Individual compounds	References
Isoflavanes	Have 3-phenylchroman backbone $C_{15}H_{14}O$	Lonchocarpane, laxiflorane, dalvelutinanes A and B, 3 (S)-3′-hydroxy-8-methoxyvestitol, nitidulan, nitidulin	Kaennakam, Siripong, and Tip-pyang (2017)
Isoflavandiols	$C_{15}H_{14}O_3$	Equol (4′,7-isoflavandiol)	Rufer, Glatt, and Kulling (2006)
Isoflavenes	Related to isoflavanes but with a double bond in ring-B	7-hydroxy-2′-methoxy-4′,5′-methylenedioxyisoflav-3-ene (judaicin), judaicin 7-*O*-glucoside, judaicin 7-*O*-(6″-*O*-malonylglucoside)	Stevenson and Veitch (1996)
Pterocarpans or Coumestans (phytoestrogens)	Polycyclic aromatic compound containing a coumestan moiety	Coumestrol, wedelolactone, demethylwedelolactone, psoralidin, flemicoumestan A 1, glycyrol, erythribyssin N, aureol, tephcalostan, plicadin, sophoracoumestan A, coumestoside C, D, hedysarum, coumestans A, B, D, F	Nehybova, Smarda, and Benes (2014)
Rotenoids	Heterocyclic aromatic compound: supplementary ring carbon atom derived from a methoxy group.	Elliptone, deguelin, malaccol, toxicarol, rotenone, sumatrol, tephrosin, amorphigenin, dolineone, pachyrrhizone, erosone	Uddin and Khanna (1979), Patil and Masand (2018)
Alkaloids			
Pyrrolidine alkaloids	Pyrrolidine or Tetrahydropyrrole ring	hygrine	Jan and Abbas (2018)
Pyridine alkaloids	Piperidine or Hexahydropyridine ring	coniine, piperine, isopelletierine	
Pyrrolidine-pyridine alkaloids	Pyrrolidine-pyridine	myosmine, nicotine	
Pyridine-piperidine alkaloids	Pyridine ring joined to piperidine ring	Anabasine	
Quinoline alkaloids	Quinolone	Quinine, anthraquinone, abruquinone	
Isoquinoline alkaloids	Isoquinoline	Opium alkaloids like narcotine, papaverine, morphine, codeine, and heroine	

whereas complex polymerized compounds (flavanols and anthocyanins) are present in wine (Fennema, 1996).

3.3.2.5 Phenolic acids

The principal phenolic acids in plants are derivatives of hydroxybenzoic acids and hydroxycinnamic acids. Hydroxybenzoic acid derivatives exist as glucoside forms, and hydroxycinnamic acids occur as esters with quinic acid or sugars (Rashmi & Negi, 2020b).

3.3.2.5.1 Derivatives of hydroxybenzoic acids

4-hydroxybenzoic acid is a monohydroxybenzoic acid in which a benzoic acid carries a hydroxy substituent at C-4 of the benzene ring, which is a conjugate acid of 4-hydroxybenzoate. Gallic acid is a trihydroxyl derivative, which may also be present in esterified form as hydrolysable or condensed tannins and their monomers. Ellagic acid exists in ellagitannins as esters of diphenic acid analog along with glucose. It is produced due to the hydrolysis of tannins such as ellagitannin and geraniin. Gentisic acid (2,5-dihydroxybenzoic acid) is a biosynthetic derivative and metabolite of salicylic acid (2-hydroxybenzoic acid) (Belles et al., 1999). It is produced by carboxylation of hydroquinone, whereas along with oxygen and enzyme gentisate 1,2-dioxygenase, gentisic acid yields maleylpyruvate (Hudnall, 2000).

Protocatechuic acids, also known as 3,4-dihydroxybenzoic acid, belonging to catechols and a dihydroxybenzoic acid, as well as conjugate acid of 3,4-dihydroxybenzoate. Syringic acid is a chemical compound naturally found as *O*-methylated trihydroxybenzoic acid. It is a derivative from gallic acid and conjugate acid of a syringate. It is synthesized by hydrolyzing eudesmic acid along with sulfuric acid. Vanillic acid (4-hydroxy-3-methoxy benzoic acid) is a dihydroxybenzoic acid derivative. Vanillic acid is the oxidized form of vanillin, and it is an intermediate in the formation of vanillin from ferulic acid (Civolani, Barghini, Roncetti, Ruzzi, & Schiesser, 2000; Lesage-Meessen et al., 1996).

3.3.2.5.2 Derivatives of hydroxycinnamic acids

Hydroxycinnamic acids include several compounds comprising a quinic acid moiety with a cyclohexane ring having four hydroxyl groups at different positions and a carboxylic acid (Alam et al., 2016; http://www.hmdb.ca/metabolites/HMDB0041641). The 3,4-Dicaffeoylquinic acid is a natural product, which is an ester of two polyphenolic caffeic acids and one cyclitol (−)-quinic acid. 3,5-Dicaffeoylquinic acid (3,5-DCQA) is a carboxylic ester that is obtained by the condensation of the hydroxy groups at positions 3 and 5 of (−)-quinic acid with the carboxy group of *trans*-caffeic acid. The 3,4-diferuloylquinic acid and 3,5-diferuloylquinic acid are insoluble in water and a weakly acidic compound (Bezerra et al., 2017; http://foodb.ca/compounds/FDB000277), whereas 3-p-coumaroylquinic acid is slightly soluble in water and a weak acidic compound. Caffeoylquinic acids (CQA) are compounds composed of a quinic acid core, acylated with one or more caffeoyl groups (Miyamae, Kurisu, Han, Isoda, & Shigemori, 2011). This class includes compounds such as Chlorogenic acid (3-*O*-caffeoylquinic acid or 3-CQA), 4-*O*-caffeoylquinic acid (crypto-chlorogenic acid or 4-CQA) and 5-*O*-caffeoylquinic acid (neo-chlorogenic acid or 5-CQA) (Wianowska & Gil, 2019). The 4-*O*-Caffeoylquinic acid (Cryptochlorogenic acid), is an isomer of chlorogenic acid, which possesses antioxidant properties. The 5-caffeoylquinic acids, an isomer of chlorogenic acid are the most important groups of phenolic secondary metabolites, which are the esters formed

between cinnamic acid derivatives and quinic acid (Clifford, 2000; Clifford, Johnston, Knight, & Kuhnert, 2004). The 4-feruloylquinic acid (*O*-feruloylquinate), 3-p-coumaroylquinic acid and 1-*O*-feruloyl glucose are slightly soluble in water and weak acidic compound (http://foodb.ca/compounds/FDB000248; http://foodb.ca/compounds/FDB000866; Li & Bet, 2013). The 1-*O*-feruloylglucose belong to the class of hydroxycinnamic acid glycosides, which are glycosylated hydoxycinnamic acids derivatives (http://foodb.ca/compounds/FDB015907). The 5-p-coumaroylquinic acid is a cinnamate ester obtained by formal condensation of the carboxy group of 4-coumaric acid with the 5-hydroxy group of (−)-quinic acid (http://foodb.ca/compounds/FDB000236). Caffeic acid (3,4-dihydroxycinnamic) is the hydroxycinnamate and phenylpropanoid metabolites more widely distributed in plant tissues (Clifford, 2000; Mattila, Hellström, & Törrönen, 2006). Cinnamic acid is the precursor for the biosynthesis of lignins, phenyl-propanoids, coumarins, tannins, flavonoids, pigments, isoflavonoids, flavonoids, stilbenes, aurones, anthocyanins, spermidines, flavor components of spices and various alkaloids such as morphine and colchicines (Vogt, 2010). Cinnamic acids are ester conjugates with quinic acid, or with other acids, sugars or lipids, or form amides with aromatic and aliphatic amines (De, Baltas & Bedos-Belval, 2011). Ferulic acid is chemically defined as ([E]-3-[4-hydroxy-3-methoxy-phenyl] prop-2-enoic acid), which are available in the plant tissues (Mattila & Kumpulainen, 2002). Sinapic acid (3,5-dimethoxy-4-hydroxycinnamic acid) is available both in the free and ester form. Hydroxycinnamic esters occur as sugar esters (glycosides), or as esters of a variety of organic compounds. There are two types of sinapoyl esters, the sinapoyl malate present in leaves, and sinapine (sinapoylcholine) stored in roots. Sinapine is an alkaloidal amine, which is a choline ester of sinapinic acid (Chapple, Vogt, Ellis, & Somerville, 1992; Shirley & Chapple, 2003).

3.3.3 Glucosinolates

Glucosinolates are sulfur- and nitrogen-containing glycosides commonly found in Brassicaceae family. The type and concentration of glucosinolates accumulated in plants depends on genotype, growing conditions, developmental stage, type of plant tissue and postharvest handling. Approximately 140 different glucosinolates have been identified in plants, which also include glucosinolate degradation products such as isothiocyanates, indoles, dithiothiols and other organosulfur compounds. Glucosinolate degradation products are well known for their antimicrobial activity (Barbieri et al., 2017) and anti-carcinogenic effects (Hayes, Kellesher, & Eggleston, 2008).

Glucosinolates consist of a β-D-glycopyranose residue linked to a hydroximinosulfate ester by sulfur bridge, and an R-group. Glucosinolates are broadly classified in three classes based on the structure of different amino acids precursors linked to the R-group, as aliphatic glucosinolates (derived from alanine, leucine, isoleucine, methionine, or valine), aromatic glucosinolates (derived from phenylalanine or tyrosine), or indole glucosinolates (derived from tryptophan). The R chains may also contain double bonds, oxo, hydroxyl, methoxy, carbonyl or di-sulfide linkages. The major glucosinolates include progoitrin, sinigrin, glucobrassican, neoglucobrassican, and glucoraphanin. The other glucosinolates metabolites include thiocyanates, nitriles, sulfates, and goitrins (Bischoff, 2006). Major glucosinolates and their derivatives are given in Table 3.5, and their chemical structures are presented in Fig. 3.4.

Table 3.5 Major glucosinolates and their derivatives in plant extracts.

Glucosinolates	Derivatives	Plant source	References
Isothiocyanate	Sinigrin precursor to allyl isothiocyanate	Mustard, broccoli, cabbage, cauliflower, kale, mustard, radish, brussels sprout, watercress	McNaughton and Marks (2003)
Gluconasturtiin (phenethylglucosinolate)	Phenethyl isothiocyanate	Cruciferous vegetables-cabbage, mustard or rapeseed	Ishida, Hara, Fukino, Kakizaki, and Morimitsu (2014), Li and Kushad (2004)
Glucobrassicin	1-Methoxyglucobrassicin (neoglucobrassicin) 4-Hydroxyglucobrassicin 4-Methoxyglucobrassicin 1,4-Dimethoxyglucobrassicin 1-Sulfoglucobrassicin 6′-Isoferuloylglucobrassicin	Horseradish, cabbage, mustard, broccoli	Agerbirk, De Vos, Kim, and Jander (2009), Galletti, Barillari, Iori, and Venturi (2006), Ishida et al. (2014)
Benzylglucosinolate (Glucotropaeolin)	Benzyl isothiocyanate (BITC)	Cruciferous vegetables, particularly garden cress	Higdon (2005), Ishida et al. (2014)
(*R*)-4-(methylsulfinyl) butylglucosinolate (Glucoraphanin)	Sulforaphane	Cruciferous vegetables mustard, broccoli and red cabbage	Ishida et al. (2014), Leicach and Chludil (2014)
(*R*)-2-hydroxybut-3-enylglucosinolate (progoitrin)	(*S*)-2-hydroxybut-3-enyl isothiocyanate, which is expected to be unstable and immediately cyclize to form (*S*)-5-vinyloxazolidine-2-thione (goitrin)	Mustard, broccoli, cabbage, cauliflower, kale, radish, brussels sprout, watercress, peanut, kohlrabi and spinach	Ishida et al. (2014), Rossiter and James (1990)
Sinalbin	4-Hydroxybenzyl isothiocyanate	Seeds of white mustard	Borek and Morra (2005), Ishida et al. (2014)

3.3.4 Other phytochemicals

Other phytochemicals in various plant extracts include Betalains, Betacyanins, Betanin, Isobetanin, Probetanin, Neobetanin, and Betaxanthins such as Indicaxanthin and Vulgaxanthin. Alkaloids contain one nitrogen atom in the form of primary, secondary, or tertiary amine. Sometimes the number of nitrogen bases may go up to five. Alkaloids have been reported to possess antimicrobial activity since ancient time. Several organic acids such as Phytic acid (Inositol hexaphosphate), Quinic acid, Oxalic acid, Tartaric acid, Anacardic acid, and Malic acid are also present in various extracts. Various plant extracts also contain Chlorophylls and Chlorophyllin, Amines such as Betaine, Choline, Carnitine, Coenzyme Q_{10}, Ubiquinone, and Ubidecarenone.

3.4 Structure-activity relationship of plant extract

The diverse nature of chemical structures in plants is related to their multifaceted properties, which is linked to their specific biological activity (Cheynier, 2012). The nature of chemicals present in plant extracts determines their biological activity. Several plant extracts obtained from grape seeds, green tea, rosemary, pomegranates and cinnamon, are found to be similar or better antioxidant compared to synthetic antioxidants (Shah, Bosco, & Mir, 2014). Some plant extracts, in addition to being antioxidant, also exhibit antimicrobial activity, and influence the textures and flavor of food (Soto-Vaca, Gutierrez, Losso, Xu, & Finley, 2012). The chemical compounds present in plant extracts varies in their structure (Figs. 3.2–3.4), and these structures influence bioactivities of plant extracts.

3.4.1 Structure-activity relationship of carotenoid

The antioxidant properties of carotenoids are related to their chemical structure. The nature of the specific end groups in carotenoids influences their polarity, which affects their interaction with biological membranes and thus antioxidant activity. Arrangement of conjugated double bonds in the carotenoids also impacts antioxidant activity. The opening of the β-ionone ring in the carotenoid structure and addition of oxygenated functional groups increase their ROO · scavenging capacity. The increase in polyene chain length also affects the quenching of singlet oxygen. Isolated double bond and lack of oxygen substituents also influences their antioxidant activity (Kobayashi & Sakamoto, 1999). The size and shape of carotenoids are important for functionality. The tendency of *cis*-isomers to crystallize is much faster that *all trans*-isomers, and are readily solubilized and transported. Therefore, the *trans* isomers are more efficient than their corresponding *cis* ones (Britton, 1995). Table 3.6 summarizes the structure activity relationship of carotenoids present in the plant extracts.

3.4.2 Structure-activity relationship of phenolics

The biological activity of phenolics is related to the presence of a 3-hydroxyl substituent, a 3′4′-dihydroxy (catechol or B ring) moiety, and the C_4 oxo group and C_2C_3 double bond. The hydroxyl groups confer antioxidant and metal chelating activity, whereas methoxy groups increase lipophilicity and membrane transport. A double bond and carbonyl functional group in the heterocycle or polymerization increases biological activity (Heim, Tagliaferro, & Bobilya, 2002). Table 3.7 summarizes the structure activity relationship of various phenolic compounds present in the plant extracts.

3.4.2.1 Antioxidant activity

Increased antioxidant potential of flavonoids is correlated to their enhanced number of hydroxyl groups. The most important structure for scavenging actions is the presence of two hydroxyl groups in the B ring at ortho position. Existence of hydroxyl groups at the positions 5, 6, and 7 in the ring A are crucial for scavenging activity. The presence of metal complexing domains between the

Table 3.6 Structural changes in carotenoids present in plant extracts and their influence on biological activities.

Structural changes	Changes in bioactivity	References
Pattern of conjugated double bonds in the polyene backbone	Antioxidant activity increases with increase in double bonds	Kobayashi and Sakamoto (1999)
Opening of the β-ionone ring	Increase of ROO· scavenging capacity	Rodrigues, Mariutti, Chiste, and Mercadante (2012)
Increase of chromophore extension	Increase of ROO· scavenging capacity	Rodrigues et al. (2012)
Addition of oxygenated functional groups	Increase of ROO· scavenging capacity	Rodrigues et al. (2012)
Increase in polyene chain length	Increase in quenching of the singlet oxygen	Krinsky (1998)
Cis-trans isomerization	*All-trans* form are more efficient ROO· scavenger than their corresponding *cis* ones	Britton (1995)
Linearity of structure	Reduced bioavailability of trans-isomers as compared to corresponding *cis* ones	Levin and Mokady (1995), Ferruzzi, Lumpkin, Schwartz, and Failla (2006)

5-hydroxyl and 4-carbonyl group, the 3-hydroxyl and 4-carbonyl group, and between the 3′,4′-hydroxyl groups are responsible for metal chelating ability of flavonoids (Sordon et al., 2016).

In general, it is considered that a higher number of hydroxyl substituents in flavonoids results in a higher antioxidant activity (Burda & Oleszek, 2001; Pietta, 2000; Rice-Evans, Miller, & Paganga, 1996). The presence of two hydroxyl groups in the ortho position of ring B is confirmed as the most important factor, although adjacent hydroxyl groups at positions 5 and 6 (and 7) in ring A may replace ring B hydroxyl groups scavenging function (Heim et al., 2002). The 3′,4′-dihydroxy-phenolic structure of ring B molecules may result in a stable radical after interaction with ROS. The removal or derivatization of one of the hydroxyl groups in the ortho position of ring B markedly decreases the ROS-scavenging activity. An additional hydroxyl group in ring B (pyrogallol structure) does not greatly influence the activity of flavonols or anthocyanins, but may increase the activity of flavanols (Rice-Evans et al., 1996).

Free radical scavenging by flavonoids is enhanced by the presence of both (2−3 double bond and 4-oxo). Conjugation between the A- and B-rings permits a resonance effect of the aromatic nucleus that stabilizes the flavonoid radical. The research reports indicate that the flavonoids devoid of 2−3 double bond and/or 4-oxy group have lower antioxidant activity than those with both the structural features (Wolfe & Liu, 2008).

Aglycones are more potent antioxidants than their corresponding glycosides. The total number, the position, and structure of the sugar play an important role. Sugar in A-ring shows higher reduction of antioxidant activity than 3-glycosylation in the heterocycle. *O*-glycosylation at carbon 7 weakens the antioxidant effect of flavonoids, however *O*-glycosylation at carbon 3 has no effect. The type of the sugar moiety also plays an important role in determining the antioxidant effect

Table 3.7 Structural changes in phenolic compounds present in plant extracts and their influence on biological activities.

Bioactive compound (s)	Structural changes	Changes in bioactivity	References
Phenolic compounds	Number of hydroxyl groups in relation to carboxyl functional group	Antioxidant activity increases with increase in hydroxyl groups	Afanasev, Dcrozhko, Brodskii, Kostyuk, and Potapovitch (1989), Amarowicz, Pegg, Rahimi-Moghaddam, Barl, and Weil (2004)
Monohydroxybenzoic acids	−OH moiety at ortho- or para-position to −COOH	No antioxidant activity	Rice-Evans et al. (1996)
Trihydroxylated gallic acid	Increase in degree of hydroxylation	Antioxidant activity increases	
Syringic acid	Replacement of hydroxyl groups at 3- and 5-position with methoxyl groups	Antioxidant potential decreases	
Hydroxycinnamic acids	CH = CH−COOH group confirmshigher H-donating capacity and radical stabilization than −COOH group	Antioxidant activity increases	Andreasen, Landbo, Christensen, Hansen, and Meyer (2001), Rice-Evans et al. (1996)
Hydroxybenzoic acids	CH = CH−COOH group endorsesreduced H-donating capability and radical stabilization than −COOH group	Antioxidant activity decreases	Andreasen et al. (2001), Rice-Evans et al. (1996)
Flavonoids	Structural features and nature of substitutions on rings B and C; Double bond between C-2 and C-3, conjugated with 4-oxo group in ring C	Antioxidant activity increases	Pietta (2000)
Catechol group	Degree of hydroxylation and sites of −OH groups in B ring (ortho-dihydroxyl structure of ring B)	Higher antioxidant activity	Pietta (2000), Van Acker et al. (1996a, 1996b)
Pyrogallol group	Presence of hydroxyl groups at 3-O-, 4-O-, and 5-O-positions of ring B	Antioxidant activity increases	Van Acker et al. (1996a, 1996b)
Anthocyanidins	Conversion of 3-O, 4-O-dihydroxyphenyl to 3-O, 4-O, 5-O−trihydroxylphenyl	Antioxidant activity increases	Seeram and Nair (2002)
Catechins	Conversion of 3-O, 4-O-dihydroxyphenyl to 3-O, 4-O, 5-O−trihydroxylphenyl	Antioxidant activity decreases	Seeram and Nair (2002)

Table 3.7 *(Continued)*

Bioactive compound (s)	Structural changes	Changes in bioactivity	References
	B-ring catechol	Antioxidant activity increases due to peroxynitrite scavenging	Kerry and Rice-Evans (1999)
Flavones	Catechol or *o*-trihydroxyl (pyrogallol)—Absent	Weak antioxidant property	Burda and Oleszek (2001), Gao, Huang, Yang, and Xu (1999), Pannala, Chan, O'Brien, and Rice-Evans (2001)
Kaempferol	Double bond between C-2 and C-3, combined with a 3-OH, in ring C	Antioxidant potential increases	Van Acker et al. (1996a, 1996b)
	Substitution of 3-OH	Antioxidant activity reduces	Seeram and Nair (2002)
Quercetin	1. o-diphenolic group (in ring B), 2. 2−3 double bond conjugated with 4-Oxo function, 3. hydroxyl groups at 3 and 5 position	High Antioxidant activity	Bravo (1998)
Luteolin	3,4-catechol structure in B-ring	Enhanced peroxyl radical scavenging ability	Van Acker et al. (1996a, 1996b)
Naringenin (4, 5, 7-trihydroxyflavanone),	Three OH substitution on structure but no 3′,4′-di-OH-structure	No influence on antioxidant activity (Heridictyol vs Naringenin)	Di Majo et al. (2005)
Heridictyol (5,7, 3,4 tetrahydroxyflavanone),	Four hydroxyl groups substitutions with 3′,4′-di-OH-structure		
Neoeriocitrin (Heridictyol-7-neohesperidoside),	Glycosylated with a neohesperidose of 7th OH group, 3′,4′-catechol structure	Increase in antioxidant activity (Neoeriocitrin vs Naringenin)	
Hesperitin (3′, 5, 7-trihydroxy-4′ methoxyflavanone)	*O*-glycosylation at hydroxyl position	Higher antioxidant activity than Neohesperidin due to steric effect disturbs the planarity and ability to delocalize electrons	
Neohesperidin (Hesperitin-7-neohesperidoside) Neoeriocitrin (Heridictyol-7-neohesperidoside)	Replace with a neohesperidoside molecule in 7th position, a methoxylation in 4th position	Decreases antioxidant power-(Neohesperidin vs Neoeriocitrin)	

(*Continued*)

Table 3.7 ***(Continued)***

Bioactive compound (s)	Structural changes	Changes in bioactivity	References
Chalcones	−SCH3 and −OCH3 in para position of A-ring and −OH in B-ring	Antioxidant activity increases	Sivakumar, Prabhakar, and Doble (2011)
Neoechinulin A	C-8/C-9 double bond forms conjugate with indole and diketopiperazine moieties of Neoechinulin A	Antioxidant activity increases	Kuramochi (2013)
	Stereo chemistry of C12	No influence on antioxidant activity	
	Presence of intact diketopiperazine moieties is requirement	No influence on antioxidant activity	
Caffeic acid derivatives	Caffeic acid anilides with electron donating groups at *p*-position	Higher inhibitory activities against *B. subtilis*	Fu, Cheng, Zhang, Fang, and Zhu (2010)
Chalcones	Lipophilicity of ring A of hydroxyl chalcones	Higher inhibitory activities against *S. aureus* and *E. coli*	Batovska et al. (2009)
4-Methoxy phenylpropanone	Introduction of keto group in place of double bond	Increased inhibitory effect against various bacterial strains	Raj, Narayana, Ashalatha, Kumari, and Sarojini (2007)
4-Methoxy phenylpropanol	Addition of alcohol group in place of double bond	Enhanced antifungal activity	Raj et al. (2007)
Polymethoxylated flavones (PMFs),	Four or more methoxyl groups on basic benzo-γ-pyrone (15 carbon, C-6 − C-3 − C-6) skeleton with a carbonyl group at C-4	Enhanced antifungal activity against *Aspergillus niger*	Liu, Xu, Cheng, Yao, and Pan (2012)
Kaempferol,	Hydroxyl group substitutions at C-3, C-5, C-7, and C-4′	Higher Anti-*E. coli* activity with substitution	Wu, Zang, He, Pan, and Xu (2013)
Nobiletin (PMF)	Methoxyl group substitutions at C-5, C-6, C-7, C-8, C-3′, and C-4′	Lowest Anti-*E. coli* activity with substitution	Constantinou et al. (1995)
Quercetin, Myricetin, and Kaempferol	C-4 keto group and hydroxyl group substitutions at C-3, C-7, and C-4′	Higher Anti-*E. coli* activity with substitution	
Flavonoids	4′-OH in B ring	Higher inhibition of influenza virus	Liu et al. (2012)
5-Hydroxyflavanones 5-Hydroxyisoflavanones	One, two, or three additional hydroxyl groups at 7, 2′, and 4′ positions	Higher inhibition of *Streptococcus mutans* and *Streptococcus sobrinus*	Osawa et al. (1992)

Table 3.7 ***(Continued)***

Bioactive compound (s)	Structural changes	Changes in bioactivity	References
Cyclic C5-curcuminoids	Changes in benzylidene group and nitrogen heteroatom	Better antiproliferative activity	Huber et al. (2020)
Seco-pseudoguaianolides paulitin and isopaulitin	Two α β unsaturated (C−O−CH = CH2) systems	Better antiproliferative activity	Chen, Liu, and Wang (2011)
Psilostachyin	Single C−O−CH = CH2 moiety in the molecule	No effect on antiproliferative activity	
Sintenin	No α β unsaturated (C−O−CH = CH2)	No effect on antiproliferative activity	
Gallic acid	Three hydroxyls and one carboxylic acid group	Higher antioxidant ability and neuroprotective effect	Lu, Nie, Belton, Tang, and Zhao (2006), Phonsatta et al. (2017), Rajan and Muraleedharan (2017)
Luteolin	OH groups at C-5, C-7, C-3′, and C-4′	Higher anti-leishmanial potential	Tasdemir et al. (2006)
7,8-Dihydroxyflavone	Basic structure	Higher anti-leishmanial potential	
7,8-Dihydroxyflavone	Addition of a catechol structure into the B ring	Diminished anti-leishmanial activity upto fivefold	
Apigenin and Luteolin	Sugars (one or more) at C-5 or the C-7 position	Reduction in anti-leishmanial potency	
3-Hydroxyflavone	Pattern of hydroxylation on ring B	Higher anti-leishmanial potential	
Fisetin	OH groups at C-3, C-7, C-3′, and C-4′	Higher anti-leishmanial potential	
Quercetin	Catechol moiety in ring B	Higher anti-leishmanial potential	
Kaempferol	*p*-Hydroxyphenyl ring	Lesser anti-leishmanial activity	
Morin	OH in *meta*-position at C-2′ and C-4′	Lesser anti-leishmanial activity	
7,8-dihydroxyflavone and 6,7-dihydroxyflavone	Hydroxylation on ring B absent, however, catechol function at side chain	Higher anti-*Trypanosoma brucei rhodesiense* activities	
Catechol, Pyrogallol, Gallic acid, and 3,4-dihydroxybenzoic acid	Two or three OH groups positioned *ortho* to each other	Significant trypanocidal activities	
Phenolic esters; Methyl, propyl and octyl esters of caffeic and gallic acids	Size, degree of ring hydroxyl substitution and length of alkyl chain, lipophilicity	Antiproliferative and/or cytotoxic activity higher than phenolic acids	Fiuza et al. (2004)

(Fennema, 1996). *O*-methylation can change hydrophobicity and impart steric effects (at the cost of OH). The suppression of antioxidant activity by *O*-methylation is attributed to the steric effects (Fennema, 1996). The protection of lipids against oxidative damage is achieved by scavenging of hydroxyl, and peroxyl, or termination of chain reactions or chelation of divalent cations, which help in reducing or recycling the flavonoid radical (Fennema, 1996).

3.4.2.2 Antimicrobial activity

The antibacterial activity of flavonoids is due to the inhibition of nucleic acid synthesis, cytoplasmic membrane function, energy metabolism, biofilm formation, and alteration of the membrane permeability. Hydroxyl groups at the special sites on the aromatic rings of flavonoids improve the antibacterial activity. The methylation of the active hydroxyl groups generally decrease the activity. The hydrophobic substituents such as prenyl groups, alkylamino chains, alkyl chains, and nitrogen or oxygen containing heterocyclic moieties usually enhance the antimicrobial activity for all the flavonoids (Xie, Yang, Tang, Chen, & Ren, 2015).

3.5 Conclusions

The plant extracts are rich in chemicals that impart them various biological activities. Plant extracts show lot of variability as the chemical compound in them are affected by cultivar of plant, growing conditions, plant part, maturity of plants, method of extraction and storage. There is a need to standardize the extract composition. The extract or dried preparation from plants may contain several chemical compounds in varied proportion, which pose a challenge for standardization of plant extracts. The plant extracts contain a diverse range of active chemicals, which include terpenoids, phenolics, flavonoids, tannins, glucosinolates, alkaloids, etc., among others. These chemical compounds are known to exert several bioactivities, such as antimicrobial, antioxidant, anticancer, antidiabetic and cardioprotective effects, and have potential for food and medicinal applications. Therefore, optimization of isolation, purification, and identification procedures that yield better functional properties of active chemical compounds from various plants are required.

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