

ISSN 2320-3862  
JMPS 2016; 4(2): 90-93  
© 2016 JMPS  
Received: 08-03-2016  
Accepted: 04-04-2016

Ram Singh  
Department of Applied  
Chemistry, Delhi Technological  
University, Delhi – 110 042,  
India.

## Chemotaxonomy: A Tool for Plant Classification

Ram Singh

### Abstract

Nature which consists of so many variabilities of living components of the environment possesses useful, harmful and inactive chemical constituents. The classification based on these chemical constituents is known as chemotaxonomy. All the living components of the environment produce secondary metabolites that are derived from primary metabolites. The chemical structure of the secondary metabolites is often specific and restricted to taxonomically related organisms. The classification of plants on the basis of specific class of secondary metabolites and their biosynthetic pathways constitutes chemotaxonomy. Its study is helpful to taxonomist, phytochemists and pharmacologists to solve selected taxonomical problems.

**Keywords:** Chemotaxonomy, Chemosystematics, Glycosides, Alkaloid, Plant phenols

### 1. Introduction

Natural Products are produced by all organisms but are mostly known from plants, insects, fungi, algae and prokaryotes. All of these organisms coexist in ecosystems and interact with each other in various ways in which chemistry plays a major role<sup>[1,2]</sup>. Many natural products are biologically active and have been used for thousands of years as traditional medicines and as natural poisons. Plants are the major contributors of natural products. Over the years, many approaches evolved towards the taxonomy of plants. These include morphological classification, anatomical classification and chemotaxonomic classification. The first two can be grouped under traditional classifications whereas the third one is modern approach to classify the plants.

The science of chemotaxonomy or chemical taxonomy is used for the classification of plants on the basis of their chemical constituents. All the living organisms produce secondary metabolites that are derived from primary metabolites. The chemical structure of the secondary metabolites and their biosynthetic pathways is often specific and restricted to taxonomically related organisms and hence useful in classification. This method of classification is considered better in comparison to traditional method due to the ease of working methodology. In this method of classification, the materials to be analyzed can be dried or crushed. The fresh or complete materials are not the compulsory requirements<sup>[3]</sup>.

The concept of chemotaxonomy has been elaborated in the past century<sup>[4]</sup>. According to De Candolle<sup>[4]</sup>.

- 1) Plant taxonomy will be the most useful guide to man in his search for new industrial and medicinal plants; and
- 2) Chemical characteristics of plants will be most valuable to plant taxonomy in the future.

Both the statements are having their importance in present day natural product studies. The rise of chemotaxonomy is mainly due to the advancement in analytical techniques for chemical analysis that can detect even trace amount of chemical compounds<sup>[5]</sup>. In plants, the more popular families that have been studied through chemotaxonomy are Malvaceae, Ranunculaceae, Magnoliaceae, Polygonaceae, and Solanaceae<sup>[6]</sup>. The findings of chemotaxonomic studies are helpful to taxonomist, phytochemists and pharmacologists to solve selected taxonomical problems.

### 2. Chemotaxonomic Classification

The phenolics, alkaloids, terpenoids and non-protein amino acids, are the four important and widely exploited groups of compounds utilized for chemotaxonomic classification<sup>[7]</sup>. These groups of compounds exhibit a wide variation in chemical diversity, distribution and function<sup>[7,8]</sup>. The system of chemotaxonomic classification relies on the chemical similarity of taxon<sup>[9,10]</sup>. Three broad categories of compounds are used in chemotaxonomy:

**Correspondence**  
Ram Singh  
Department of Applied  
Chemistry, Delhi Technological  
University, Delhi – 110 042,  
India.

primary metabolites; secondary metabolites and semantices.

## 2.1 Primary metabolites

Primary metabolites are the compounds that are involved in the fundamental metabolic pathways. Most of the primary metabolites are of universal occurrence and utilized by the plant itself for growth and development<sup>[11,12]</sup>. These compounds are ubiquitous in nature and hence play little role in chemotaxonomic classification. However, these molecules sometimes serve as useful chemotaxonomic behavior on the basis of their quantities. For example, carbohydrate sedoheptulose (Figure 1) is present in genus *sedum* in large quantity. Therefore, the accumulation of sedoheptulose in the species of genus *sedum* serves as a useful chemical character in chemotaxonomy<sup>[11]</sup>.

The water soluble polysaccharides (WSP) are also used as chemotaxonomic markers. The gas liquid chromatographic analysis on WSP from annatto tree (*Bixa orellana* L.) showed hemispherical type contained 38% rhamnose, while conical and ovate types contained 17% and 34% glucose, respectively. Thus, glucose and rhamnose content of WSP could be used to distinguish the three landraces of annatto trees<sup>[13]</sup>.

## 2.2 Secondary metabolites

Secondary metabolites are the compounds that usually perform non-essential functions in the plants<sup>[11]</sup>. They are used for protection and defense against predators and pathogens. These compounds are of restricted occurrence and hence very useful for chemotaxonomic classification. Some of the major group of secondary metabolites includes glycoside, alkaloid, volatile oil, flavonoid, plant phenols and terpenoids.

### 2.2.1 Glycosides in chemotaxonomy

Glycosides are the compounds in which one or more sugars are combined with non-sugar molecules through glycosidic linkage. Based on the linkage, the glycosides are grouped as O-glycoside, C-glycoside, N-glycoside and S-glycoside. The distribution of O-glycosides like rhein is very common, so it has little chemotaxonomic value. The *R. rugosa* flavonol glycosides were shown to be important chemotaxonomic markers for the classification of species in Cinnamomeae<sup>[14]</sup>. The use of flavonol glycosides as chemotaxonomic markers could be useful for the identification of *Rosa* species belonging to sections Gallicanae, Cinnamomeae, Caninae, and Synstylae<sup>[14]</sup>. The C-glycosides like aloin, cascaroside which possess a direct carbon linkage between sugar and non-sugar are not very prevalent in nature. They are found in some plants containing anthraquinone derivatives<sup>[15,16]</sup> such as aloin in aloe-liliaceae<sup>[17,18]</sup> cascaroside in cascara-rhamnaceae (Figure 2)<sup>[19]</sup>. S-Glycosides Sinigrin are exemplified by those produce isothiocyanate on hydrolysis. These compounds are characteristic of the family cruciferae, moringaceae, capparaceae. So these families have phylogenetic relationship<sup>[20]</sup>.

### 2.2.2 Cyanogenic glycoside in chemotaxonomy

The cyanogenic glycosides are the compounds responsible for providing defensive mechanism to plants<sup>[11]</sup>. Plant species have ability to produce hydrogen cyanide (HCN) by enzymatic hydrolysis of cyanogenic glycosides by the process called cyanogenesis<sup>[21]</sup>. Cyanogenesis is reported for the first time in the genera *Beilschmiedia*, *Cardwellia*, *Cleistanthus*, *Elaeocarpus*, *Embelia*, *Mischocarpus*,

*Opisthiole*, *Parsonsia* and *Polyscias*<sup>[22]</sup>. Different amino acid like phenyl alanine, tyrosine, valine, leucine, and isoleucine are precursor for the biosynthesis of cyanogenic glycosides, but they are restricted to particular family. For example, a cyanogenic glycoside synthesized from leucine commonly occurs in the subfamily amygdaloideae (almond) and maloideae (apple) of family rosaceae<sup>[11]</sup>. The glycosides derived from tyrosine commonly occur in the families of the order mangnoliales and laurales<sup>[11]</sup>.

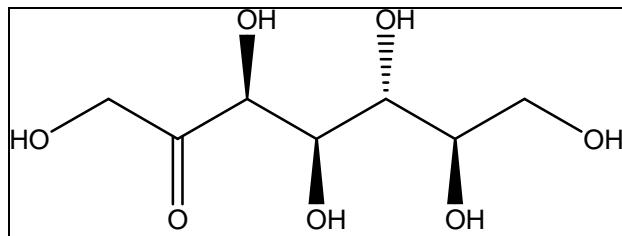


Figure 1: Sedoheptulose

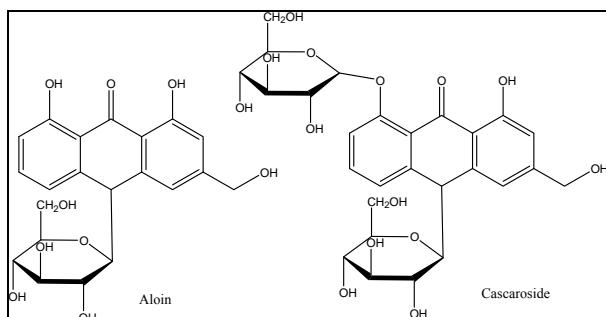


Fig 2: Aloin and Cascaroside

### 2.2.3 Glucosinolates in chemotaxonomy

Glucosinolates are sulfur- and nitrogen-containing plant secondary metabolites common in the order Capparales, which includes the Brassicaceae family (Figure 3)<sup>[23]</sup>. On the basis of alkyl component of glucosinolate compound, brassica species can be differentiated. For example, *Brassica juncea* (mustard) from Indian subcontinent contain 3-butetyl glucosinolate and allylglucosinolate while those from Asiatic country contain only allyl compound<sup>[24,25]</sup>. So, ancestry of Indian species is doubtful, because that is the hybrid of *B. nigra* (allylglucosinate) and *B. campestris* (3-butetyl glucosinate).

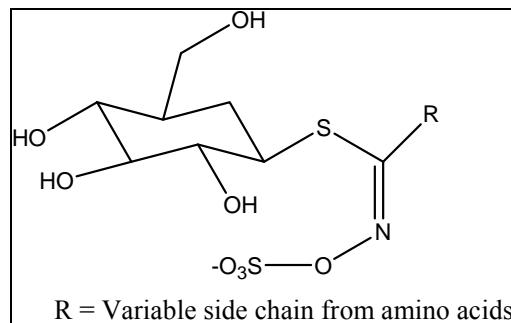


Fig 3: Glucosinolates

### 2.2.4 Alkaloid in Chemotaxonomy

Alkaloids are heterocyclic nitrogen containing basic compounds<sup>[26,27]</sup>. But, few non-heterocyclic alkaloids are also present. Chemotaxonomic analysis based on alkaloids depends upon the type of parent base compound present in the alkaloids. The indole alkaloids contain indole as the

parent base. More than 2,500 indole alkaloids were isolated mainly from three plant families, Rubiaceae, Loganiaceae and Apocynaceae. These are formed from two building blocks secologanin and tryptamine or tryptophane through a single precursor, strictosidine, and suggesting relationship between these families<sup>[28,29]</sup>. Other indole alkaloids like physostigmine (Figure 4) obtained from *Physostigma venenosum* (family Leguminosae)<sup>[30]</sup> yohimbine from *Rauvolfia serpentine* (family Apocynaceae)<sup>[31]</sup>, and *corynanthe yohimbe* (family Rubiaceae)<sup>[32]</sup> and Vinblastine from *vincarosea* (family Apocynaceae)<sup>[33]</sup>.

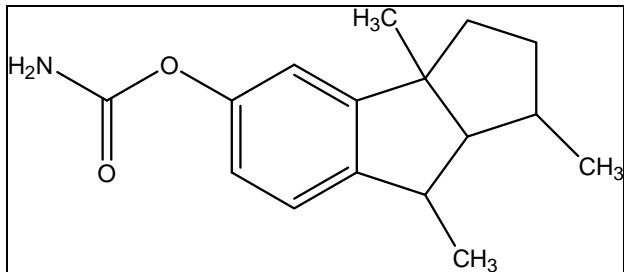


Fig 4: Physostigmine

The Pyridine and Piperidine alkaloids like Lobeline obtained from *Lobelia inflata* family Lobeliaceae<sup>[34]</sup>. Nicotine obtained from *Nicotiana tabacum* family Solanaceae<sup>[35]</sup>. Anabasine obtained from *Nicotiana glutinosa* family Chenopodiaceae<sup>[36]</sup>. The presence of these alkaloids explains the importance of these alkaloids in taxonomical analysis. Anabasine occurs in tobacco, where it is formed from lysine and nicotinic acid, whereas in the legume and chenopod species this can be synthesized from two molecules of lysine<sup>[36]</sup>. Similarly, the alkaloids like isoquinoline alkaloids, tropane alkaloids, indole alkaloids etc have also been a useful tool for taxonomic classification of plants<sup>[37]</sup>.

### 2.2.5 Plant Phenol in chemotaxonomy

Polyphenols are among the most widespread class of metabolites in nature, and their distribution is almost ubiquitous. It is estimated that 100,000 to 200,000 secondary metabolites exist<sup>[38]</sup> and some 20% of the carbon fixed by photosynthesis is channeled into the phenylpropanoid pathway, thus generating the majority of the naturally occurring phenolics<sup>[38,39]</sup>. Flavonoids are largest group of phenolic compounds. They are mostly found in the vacuole of higher plant and absent in lower plant. Different classes of plant phenols include flavones, flavanones, isoflavanones, isoflavonoids, anthocyanidins and chalcones. All flavonoids have common biosynthetic origin and therefore it possess the same basic structural element. For example, 2-phenylchromone skeleton. They may be present in many classes depending on degree of oxidation of pyran ring which may be open and cyclize into furan ring, e.g. 2-phenyl benzopyrilium: anthocyanin and 2-phenyl chromone: flavone, flavanol, isoflavone<sup>[40]</sup>. A chemotaxonomic study of practically all the species of the genus *Aloe* showed that flavonoids occur as major compounds in 31 out of a total of 380 species investigated<sup>[41]</sup>.

### 3. Summary

With the advancement of analytical techniques, today so many groups of plants are there in which phytochemical data has contributed to extensive taxonomic improvements. The presence or absence of a particular phytochemical in a plant along with the knowledge of its biochemical synthetic

pathways can be used to assign its taxonomic position.

**4. Acknowledgments** - The author is grateful to Council of Scientific & Industrial Research (CSIR), India, for financial support.

### 5. References

1. Reynolds T. The evolution of chemosystematics. *Phytochemistry* 2007; 68:2887-2895.
2. Larsen TO, Smedsgaard J, Nielsen KF, Hansen ME, Frisvad JC. Phenotypic taxonomy and metabolite profiling in microbial drug discovery. *Natural Product Report* 2007; 22:672-695.
3. Ankanna S, Suhrulatha D, Savithramma N. Chemotaxonomical studies of some important monocotyledons. *Botany Research International* 2012; 5:90-96.
4. De Candolle AP. *Essais sur les propriétés médicinales des plantes, comparées avec leurs formes extérieures et leur classification naturelle*, Second Edition, Paris, 1816.
5. Bhargava VV, Patel SC, Desai KS. Importance of terpenoids and essential oils in chemotaxonomic approach. *International Journal of Herbal Medicine*. 2013; 1:14-21.
6. Sivarajan VV. *Introduction to the Principles of Plant Taxonomy*, Cambridge University Press, 1991.
7. Smith PM. *The Chemotaxonomy of plants* London, Edward Arnold, 1976.
8. Hegnauer R. Phytochemistry and plant taxonomy—an essay on the chemotaxonomy of higher plants. *Phytochemistry* 1986; 25:1519-1535.
9. Atal CK. *Cultivation and utilization of aromatic plants*, 1st ed, Council of Scientific and Industrial Research, New Delhi, 1982, 15-21.
10. Rasool R, Ganai BA, Akbar S, Kamili AN, Masood A. Phytochemical screening of *Prunella vulgaris* L. - an important medicinal plant of Kashmir. *Pakistan Journal of Pharmaceutical Science*. 2010; 23:399-402.
11. Singh P. *An introduction to biodiversity*, Ane Books Pvt Ltd, 2010, 51.
12. Singh P. *Plant taxonomy: past, present and future*, edited by R Gupta, TERI, 2012, 233.
13. Parimalan R, Mahendranath G, Giridhar P. Analysis of water soluble polysaccharides as a potential chemotaxonomic marker for landraces in *Bixa orellana*. *Indian Journal of Biochemistry and Biophysics*. 2014; 51:81-86.
14. Sarangawa O, Kanazawa T, Nishizawa M, Myoda T, Bai C, Yamagishi T. Flavonol glycosides in the petal of *Rosa* species as chemotaxonomic markers. *Phytochemistry* 2014; 107:61-68.
15. Singh R, Geetanjali, Chauhan SMS. 9, 10-Anthraquinones and other biologically active compounds from the Genus *Rubia*. *Chemistry and Biodiversity* 2004; 1:1241-1264.
16. Singh R, Geetanjali. Isolation and synthesis of anthraquinones and related compounds of *Rubiacordifolia*. *Journal of Serbian Chemical Society*. 2005; 70:937-942.
17. Chiang HM, Lin YT, Hsiao PL, Su YH, Tsao HT, Wen KC. Determination of marked components - aloin and aloe-emodin - in *Aloe vera* before and after hydrolysis. *Journal of Food Drug Analysis*. 2012; 20:646-652.
18. Grün M, Franz G. In vitro biosynthesis of the C-glycosidic bond in aloin. *Planta* 1981; 152:562-564.

19. Fairbairn JW, Simic S. Vegetable purgatives containing anthracene derivatives: Part XI. Further work on the aloin-like substance of *Rhamnuspurshiana* DC. *Journal of Pharmacy and Pharmacology* 1960; 12:45T-51T.
20. Kim SJ, Kawaguchi S, Watanabe Y. Glucosinolates in vegetative tissues and seeds of twelve cultivars of vegetable turnip rape (*Brassica rapa* L.). *Soil Science and Plant Nutrition* 2003; 49:337-346.
21. Conn EE. The Metabolism of a Natural Product: Lessons Learned from Cyanogenic Glycosides. *Planta Medica* 1991; 57:S1-S9.
22. Miller RE, Jensen R, Woodrow IE. Frequency of cyanogenesis in tropical rainforests of far North Queensland, Australia. *Annals of Botany* 2006; 97:1017-1044.
23. Redovnikovic IR, Glivetic T, Delonga K, Vorkapic-Furac J. Glucosinolates and their potential role in plant. *Periodicum Biologorum* 2008; 110:297-309.
24. Barillari J, Cervellati R, Paolini M, Tatibouët A, Rollin P, Iori R. Isolation of 4-methylthio-3-butenyl glucosinolate from *Raphanussativus* sprouts (kaiware daikon) and its redox properties. *Journal of Agricultural and Food Chemistry*. 2005; 53:9890-9896.
25. Frank N, Dubois M, Goldmann T, Tarres A, Schuster E, Robert F. Semiquantitative analysis of 3-butenyl isothiocyanate to monitor an off-flavor in Mustard seeds and Glycosinolates screening for origin identification. *Journal of Agricultural and Food Chemistry*. 2010; 58:3700-3707.
26. Saxena M, Saxena J, Nema R, Singh D, Gupta A. Phytochemistry of medicinal plants. *Journal of Pharmacognosy and Phytochemistry*. 2013; 1:168-182.
27. Singh R, Geetanjali, Singh V. Exploring alkaloids as inhibitors of selected enzymes. *Asian Journal of Chemistry*. 2011; 23:483-490.
28. Szabó LF. Molecular evolutionary lines in the formation of indole alkaloids derived from secologanin. *ARKIVOC*, 2008, 167-181.
29. Szabó LF. Rigorous biogenetic network for a group of indole alkaloids derived from strictosidine. *Molecules* 2008; 13:1875-1896.
30. Mukherjee PK, Kumar V, Mal M, Houghton PJ. Acetylcholinesterase inhibitors from plants. *Phytomedicine* 2007; 14:289-300.
31. Bader FE, Dickel DF, Schlittler E. *Rauwolfia* Alkaloids. IX. Isolation of Yohimbine from *Rauwolfia serpentine*Benth. *Journal of American Chemical Society*. 1954; 76:1695-1695.
32. Singh AP, Singh R. Potent natural aphrodisiacs for the management of erectile dysfunction and male sexual debilities. *Frontiers in Bioscience* 2012; 1:167-180.
33. Kramers MR, Stebbings H. The insensitivity of Vincarosea to vinblastine. *Chromosoma* 1977; 61:277-287.
34. Yonemitsu H, Shimomura K, Satake M, Mochida S, Tanaka M, Endo T, *et al.* Lobeline production by hairy root culture of *Lobelia inflata* L. *Plant Cell Report* 1990; 9:307-310.
35. Shi Q, Li C, Zhang F. Nicotine synthesis in *Nicotianatabacum* L. induced by mechanical wounding is regulated by auxin. *Journal of Experimental Botany*. 2006; 57:2899-2907.
36. Steenkamp PA, van Heerden FR, van Wyk BE. Accidental fatal poisoning by *Nicotianaglauca*: identification of anabasine by high performance liquid chromatography/photodiode array/mass spectrometry. *Forensic Science International* 2002; 127:208-217.
37. Bentley KW.  $\beta$ -Phenylethylamines and the isoquinoline alkaloids. *Natural Product Report* 1992; 9:365-391.
38. Metcalf RL. Plant volatiles as insect attractants, CRC Crit. Rev. Plant Science 1987; 5:251-301.
39. Ralston L, Subramanian S, Matsuno M, Yu O. Partial reconstruction of flavonoid and isoflavonoid biosynthesis in yeast using soybean type I and type II chalconeisomerases. *Plant Physiology* 2005; 137:1375-1388.
40. Wink M, Waterman P. Chemotaxonomy in relation to molecular phylogeny of plants. In: "Biochemistry of plant secondary metabolism" (M. Wink, ed.), Sheffield Academic Press and CRC Press. Annual Plants Review 1999; 2:300-341.
41. Viljoen AM, van Wyk BE, van Heerden FR. Distribution and chemotaxonomic significance of flavonoids in *Aloe* (Asphodelaceae) *Plant Systematics and Evolution* 1998; 211:31-42.