

CHEMICAL CHARACTERS IN PLANT TAXONOMY: SOME POSSIBILITIES AND LIMITATIONS

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INTRODUCTION

Chemical plant taxonomy or chemotaxonomy of plants may be defined as a scientific investigation of the potentialities of chemical characters for the study of problems of plant taxonomy and plant phylogeny. Plant taxonomy is the science of delimiting, describing and naming appropriately taxa† and arranging them in a natural system of plants.

Principles of chemotaxonomy were elaborated in the past century by A. P. De Candolle¹ and by Greshoff². De Candolle put forward two postulates: (i) Plant taxonomy will be the most useful guide to man in his search for new industrial and medicinal plants; (ii) Chemical characteristics of plants will be most valuable to plant taxonomy in the future.

While the first postulate of De Candolle proved to be extremely fruitful and has been applied repeatedly when new sources of promising plant constituents are to be detected, his second postulate came to be accepted very slowly. Researchers like Rochleder³, Greshoff⁴, Rosenthaler⁵, Baker and Smith⁶, Wheldale⁷, Iwanow⁸, Colin⁹, Molisch¹⁰, McNair¹¹ and Weevers¹² were enthusiastic but rather isolated workers in the field of chemotaxonomy.

However, the fact that the first postulate of De Candolle was applied very successfully by generations of phytochemists forms an indirect proof of the validity of his second postulate. Some examples may serve to illustrate just the services plant taxonomy renders to chemists interested in distinct types of plant constituents. When the pharmaceutical industry became interested in plant steroids as starting materials for hormone synthesis, the search for suitable sources was essentially guided by taxonomic concepts. The genus *Strophanthus* was investigated first for cardenolides and its species proved, without exception, to accumulate members of this category of phytoconstituents. Thousands of species were screened for steroidal saponogens and in the taxa already known to contain them, *i.e.* in *Agavaceae*, *Dioscoreaceae* and *Liliaceae*, by far the highest frequency of occurrence was observed. In recent years the pregnane-derived alkaloids have begun to attract attention. Such alkaloid-like substances had been known for several years to be present in the apocynaceous genus *Holarrhena*. In this instance too, an alliance of genera included by taxonomists in the plant family *Apocynaceae* proved to be most promising for exploration. Very recently

† Taxon (plural: taxa) is the name for a taxonomic entity of unspecified rank; *i.e.* the term may be applied to any systematic entity (species, genus, family, etc.).

interest has developed in the steroidal alkaloids of *Buxus sempervirens* L. Quite logically other species of *Buxus* and other genera of the small family of *Buxaceae* were explored for the same type of alkaloid-like substances. We are not surprised that such compounds were indeed detected in the genera *Pachysandra* and *Sarcococca* in spite of the fact that their species look quite different from *Buxus sempervirens*, the original source of this type of alkaloid-like substances. In my opinion, such a finding is a tribute to the work of generations of taxonomists endeavouring to elaborate a natural system of plants.

Of course, there are many not yet fully understood irregularities in the distribution of plant constituents. Steroidal sapogenins occur, e.g., in some genera of *Leguminosae*, *Solanaceae* and *Zygophyllaceae*, taxa which are distinctly not related to *Liliiflorae* and cardenolides are very erratically distributed over angiospermous plants. The famous French school of heteroside chemists founded by Bourquelot has detected many cases of sporadic occurrences of glycosides during the first four decades of this century. The intensive study of the causes of melanogenesis in fading plant tissues demonstrated, for instance, that this phenomenon may be caused in non-related taxa by one and the same constituent. Arbutin [*Ericaceae*, *Proteaceae*, species of *Pyrus* (*Rosaceae*), species of *Bergenia* (*Saxifragaceae*), *Lathyrus niger* (*Leguminosae*), some species of *Rubiaceae*] and aucubin [e.g. *Aucuba* (*Cornaceae*), *Eucommiaceae*, *Globulariaceae*, *Plantaginaceae*, *Scrophulariaceae*] are good examples of relatively wide-spread plant chromogenes. These facts led Bridel and Kramer¹³ to deny any relationship between plant morphology and plant metabolism. After having isolated phlorizin from leaves of *Kalmia latifolia* (*Ericaceae*) they declared "il est intéressant de faire ressortir que le phlorizoside qui, jusqu'ici était regardé comme un principe spécifique de l'écorce de quelques Rosacées se rencontre également dans les feuilles et les fleurs de deux Ericacées, famille très éloignée des Rosacées au point de vue botanique. Cela prouve qu'ils n'existent guère des rapports entre les caractères botaniques et la composition chimique des plantes. D'autres exemples récents, notamment ceux qu'on tire de la répartition dans le règne végétal du monotroposide, de l'aucuboside, de l'arbutoside et du picéoside, viennent renforcer cette opinion".

Contrary to this statement I expect chemical characters to be as valid in future for taxonomic work as are morphological ones. To reach this stage, however, our knowledge about plant metabolism and its resulting products still has to be considerably extended.

In traditional plant taxonomy the totality of morphological characters has always to be weighed and checked carefully when decisions with regard to delimitations and classification have to be made. For instance, Symptetal is believed to be a most important character in dicotyledons but far less so in monocotyledons. The density and nature of the indument is a reliable taxonomic character in one group of plants but not at all in another. The same holds good for the structure of fruits and subterraneous organs and many other morphological characters. In taxonomy, generally, not one or a few characters but the total look of a taxon is most important. To this integral picture, without any doubt, metabolism contributes too. In my opinion, the answer given by Colin⁹ as to which types of characters may be

CHEMICAL CHARACTERS IN PLANT TAXONOMY

most useful for the study of problems of plant taxonomy can be accepted without restriction. He stated "Cela dépend sans doute du génie de la famille, comme disait Adanson, à qui l'on fait injure en s'appliquant à le disculper d'avoir méconnu le principe de la subordination des caractères . . ."

For most chemical characters, however, the overall information available at present does not yet suffice for a correct appreciation of their real contribution to the total look of a taxon. Therefore it is still impossible to judge appropriately their taxonomic importance. In many instances, of course, the taxonomic potentialities of chemical characters are seemingly apparent already.

SOME TAXONOMIC POSSIBILITIES OF CHEMICAL CHARACTERS

Chemical Characters as guides for classification

The position of many taxa in the natural system of plants is still highly uncertain. This applies to all levels of taxonomic categories, e.g. species in a genus (example: *Matricaria inodora* L. in *Matricaria*, *Chrysanthemum* or *Tripleurosperum*), genera in a family (examples: *Morina* in *Dipsacaceae*; *Toricellia* and *Corokia* in *Cornaceae*), families in an order (examples: *Hippuridaceae* in *Haloragales*; *Adoxaceae* in *Dipsacales*) and even orders in a class (example: *Taxales* in *Coniferopsida*). I chose three families of flowering plants to illustrate this point; the position attributed to them in 6 recent systems of angiosperms is given in *Table 1*.

Table 1. Position of three families in six recent systems of dicotyledons

Family	Placed in the following orders by:					
	Wettstein ¹⁴	Pulle ¹⁵	Cronquist ¹⁶	Hutchinson ¹⁷	Takhtajan ¹⁸	Engler's ¹⁹ Syllabus
<i>Callitrichaceae</i>	Tricoccae	Callitrichales	Haloragales	Lythrales	Tubiflorae- Lamiales	Tubiflorae- Verbenineae
<i>Cornaceae</i>	Umbelliflorae	Apiales (= Umbelliflorae)	Cornales*	Araliales†	Cornales§	Umbelliflorae
<i>Hippuridaceae</i>	Myrtales	Hippuridales	Haloragales	Lythrales‡	Myrtiflorae- Haloragales	Myrtiflorae- Hippuridineae

|| Derived from Solanales (= Tubiflorae).

* Not allied to Umbelliflorae.

† *Araliaceae* but not *Umbelliferae* are included in this order.

‡ *Hippuris* is included in *Haloragaceae* by Hutchinson.

§ Preceding Araliales sensu Takhtajan (i.e. *Araliaceae* and *Umbelliferae*).

Varying interpretation and evaluation of morphological characters very often result in disagreement regarding classification. In such instances taxonomists as a rule look for characters other than morphological ones (see for instance Thorne²⁰, Benson²¹, Davis and Heywood²²). Generally anatomical (Solereider²³, Metcalfe and Chalk²⁴, Carlquist²⁵), embryological (Maheshwari²⁶), palynological (Wodehouse²⁷, Erdtman²⁸) and cytological (Darlington²⁹, Manton³⁰) characters are considered first. Sometimes they produce convincing evidence and sometimes they fail to do so.

In such situations chemical characters may become very useful guides to taxonomists. At present one important task of chemotaxonomy consists in procuring additional evidence in all cases of obscure relationships of plants.

I should like to illustrate this further for the three families already mentioned in *Table 1*. *Table 2* summarizes the principal present-day knowledge concerning their constituents.

Table 2. Some constituents of three families of plants of obscure relationship

<i>Taxon</i>	<i>Iridoid Heterosides*</i>	<i>Principal sugars (vegetative organs)*</i>	<i>Principal phenolic compounds</i>
<i>Callitrichaceae</i>	aucubin, catalpol	sucrose	flavones (probably); caffeic acid
<i>Cornaceae</i> :			
<i>Aucuba</i>	aucubin	sucrose	flavonols (probably); caffeic acid
<i>Cornus</i>	cornin	glucose, sucrose	flavonols; gallic and ellagic acids; leucoanthocyanins
<i>Corokia</i>	cornin	sucrose	leucoanthocyanins
<i>Grieselinia</i>	not present	sucrose	caffeic acid; flavonols
<i>Mastixia</i>	loganin, loganic acid	glucose, sucrose	caffeic acid
<i>Hippuridaceae</i>	aucubin, catalpol	stachyose	caffeic and ferulic acids; kaempferol and scopoletin (probably)

*For most of the observations reported in these columns I am obliged to my collaborators Miss Fikenscher and Mr. Wiewfering.

A glance at *Tables 1 and 2* demonstrates distinctly that in all instances chemical characters agree well with proposals already put forward by some taxonomists.

Callitrichaceae and *Hippuridaceae* fit chemically very well in the alliance of *Tubiflorae* (compare proposal of Pulle) and differ fundamentally from members of *Myrtiflorae* (including *Haloragales* and *Lythrales*).

Cornaceae represent perhaps a rather heterogeneous family³¹. As far as chemical information is available the latter indicates a rather intimate relationship with the saxifragaceous stock and the sympetalous families of the orders *Contortae* and *Rubiales*. This makes rather acceptable an intermediate position between *Saxifragales* (or *Rosales*) and *Contortae-Rubiales* for *Cornaceae* and allied families and points distinctly against an association with *Araliaceae* and *Umbelliferae*^{31,32}. Direct derivation of *Cornales* from *Rosales* was proposed by Cronquist¹⁶.

It is my viewpoint that in every instance, where fundamental disagreements regarding relationship and classification of taxa exist between experienced taxonomists, thorough phytochemical investigations may result in a better understanding and a re-evaluation of all available facts. In this respect I should like to draw your attention to the monotypic genus *Simmondsia* which is usually, but doubtfully, included in the already mentioned family of *Buxaceae*. If a chemist were to investigate the alkaloids present in *Simmondsia californica* Nutt. he would render a most valuable service to plant taxonomy.

Chemical characters as aids in delimitations

Taxonomists endeavour to delimit taxa in such a manner that they really represent natural entities. In many instances, however, it is far from easy to

conceive true naturalness, *i.e.* to grasp "le génie du taxon". To illustrate this point I would like to summarize two different concepts of liliaceous and amaryllidaceous plants. Traditionally *Liliaceae* are characterized by having hypogynous flowers with a showy perianth, 3 + 3 stamina and a pistillum composed of 3 carpels and *Amaryllidaceae* are separated from *Liliaceae* by their epigynous flowers. Hutchinson¹⁷, however, believes that the most essential character of true amaryllidaceous plants is their umbellate inflorescence subtended by involucre bracts. This results, *e.g.*, in transferring *Allium* and allied genera, which all possess hypogynous flowers from *Liliaceae* to *Amaryllidaceae*. The delimitation of the two families was rather profoundly altered by the new concept which has been accepted by several modern taxonomists and rejected by others. The question rises, which of the two concepts results in a more natural delimitation of the two families. In such instances chemical characters may aid taxonomists in finding the best answer. With regard to the example mentioned, present-day chemical evidence favours the traditional delimitation of *Liliaceae* and *Amaryllidaceae* with respect to *Allium* and related genera because the highly characteristic alkaloids of all true amaryllidaceous plants are seemingly lacking in the *Allium* alliance and because steroidal sapogenins so wide-spread in *Liliaceae*, but apparently lacking in true *Amaryllidaceae*, do occur in *Allium* and allied genera. It is interesting to note that plant rusts seem to hold the same opinion; species attacking *Asparagus*, a liliaceous plant, attack also *Allium* but seem not to attack amaryllidaceous plants³³. This, however, may not be an independent piece of evidence since host preference of parasites may largely be governed by the chemistry of the hosts' tissue.

Chemical characters as aids in unambiguous identifications of plants

Plant species are composed of interbreeding populations of individuals. If a species has been highly successful and covers a large area at present, many of its populations become geographically and (or) ecologically separated. Gradually the gene pools of radiating populations may change and distinct topotypes or ecotypes may emerge. The latter may still be interfertile with all other populations of the species and clearly represent only variants of one wide-spread species. If, however, by polyploidy or some other mechanism barriers to gene exchange between the diverging entities have arisen or if clearcut morphological differences have evolved the matter of species delimitation becomes a delicate and difficult task. Many of the so called species aggregates have been taxonomically interpreted in different ways and nomenclature has often become complex and rather disappointing in such notoriously difficult groups. In this field of taxonomy cytotaxonomical research has proved to be often successful. It may be an invaluable aid for an unambiguous identification of distinct entities and in many instances it has offered even a clue for a better understanding of the past history of such puzzlingly complex aggregates. Frequently past history gave rise to slightly differing metabolic patterns in members of a species aggregate. The study of their chemical constituents may therefore bring to light new

characteristics helpful in identification. It is evident that each botanical study concerning present-day distribution, ecological preferences and past history of members of an aggregate species or of several closely related species of a genus depends on the unambiguous identification of each available specimen. Unfortunately morphological characters are often rather vague and cytological work is restricted to living plants. Moreover clearcut distinctive morphological characters may be restricted to organs many often lacking in the available plant specimens. *Nasturtium officinale* R.Br. and *Nasturtium microphyllum* (Boenningh.) Rchb., for instance, can only be identified with certainty if mature fruits and seeds are present and the three sub-species of *Sparganium erectum* L. are identifiable by their fruits only. A thorough study of the chemistry of each member of such aggregates and the elaboration of analytical methods which may be performed even with herbarium specimens can be, in many instances, useful to plant taxonomy. I like to illustrate this aspect by an example, with which I have some personal experience. The species of ferns generally known as *Dryopteris filix-mas* (L.) Schott is a rather complex aggregate. The cytogenetical work of Manton³⁰ has shown it to comprise essentially three well defined entities in Europe, a fertile diploid called *Dryopteris abbreviata* Lamk. et DC., a fertile tetraploid called *Dryopteris filix-mas* (L.) Schott sensu stricto and an apogamous diploid or triploid called *Dryopteris borrieri* Newm. Since several years we have investigated European species of *Dryopteris* for the phenolic compounds present in their rhizomes. Aided by Dr. J. Sundman and Miss A. Penttilä of Helsinki, who have studied intensively the chemistry of fern phloroglucides during recent years, we were able to show that the three members of the *filix-mas* aggregate differ distinctly in the composition of their phloroglucides. If adequately collected herbarium specimens are available these chemical characters can be very helpful in an unambiguous identification of dried plants, which have lost part of their morphologically most distinctive features.

There are, however, many more aspects, which make the study of chemical characters at infraspecific and specific levels a very fascinating one. Besides being helpful with the identification of plant specimens it informs us about patterns of chemical variation within genera and aggregate species and it may ultimately demonstrate how one pattern of plant constituents evolved from a preceding one. Moreover, joint botanical and phytochemical studies may provide us with a better understanding of the biological and ecological meaning of distinct spectra of primary and secondary plant metabolites. A thorough knowledge in these fields is essential for a judgement of the overall taxonomic implications of the overwhelming multitude of phytochemical patterns.

SOME FACTORS WHICH LIMIT THE TAXONOMIC VALUE OF CHEMICAL CHARACTERS

To make the most appropriate use of chemical characters in plant taxonomy one has to realize clearly that several factors affect and restrict their taxonomic meaning. I would like to discuss especially parallelism and diversification and methods of documentation.

Parallelism and diversification

Every taxonomist is aware of the fact that morphological similarity of plants does not always indicate close relationship and that, on the other hand, striking dissimilarities can often be noted between taxa supposed to be closely related. These phenomena known as parallelism (convergence) and diversification (divergence) are very often responsible for difficulties and artificialities in classification. For taxonomists who endeavour to construct a natural system of plants it is most essential to analyze carefully each instance of suspected parallelism or diversification. As these phenomena often affect morphological characters it can be taken for granted that the same holds good for chemical characters. They too are in need of a careful analysis. First of all we should be able to discern true convergence from cases of pure analogy and true divergence from cases of clearcut homology. The already mentioned plant chromogenes arbutin and aucubin may serve to illustrate these points.

At present arbutin is known to occur in a number of plant families, some of which are distinctly not closely related to the other ones (*Table 3*).

Table 3. Some of the plant families in which arbutin has been found to occur

<i>Family</i>	<i>Remarks</i>
Ericaceae	} Possibly remotely related to the rosaceous stock ----- Families related by descent ("Rosaceous stock") ----- } Possible remotely related to the rosaceous stock
Leguminosae	
Rosaceae	
Saxifragaceae	
Rubiaceae	} Possible remotely related to the rosaceous stock
Proteaceae	
Liliaceae	{ Distinctly non-related with the above-mentioned families

We need information concerning the biogenetical pathways giving rise to arbutin in *each* taxon known to accumulate this glucoside. If the pathway is the same in different taxa which are definitely non-related by a number of other criteria, then we have a clearcut example of convergence, i.e. convergent evolution. If, however, the pathway is a different one, arbutin accumulation in those taxa using a deviating pathway becomes a case of analogy; apparently the character is the same but it is acquired along different lines. It is obvious that analogous characters are of no value as guides for classification and that true convergence represents one of the many factors which make so difficult the design of a truly natural system of plants. At the same time we note that chemical parallelism may be achieved by two different processes with different taxonomic implications.

Aucubin and many closely related iridoid glycosides are especially widespread in *Saxifragaceae*, *Cornaceae*, *Garryaceae*, *Ericaceae*, *Oleales*, *Gentianales*, *Tubiflorae*, *Plantaginales* and *Dipsacales* (orders according to Engler's Syllabus). In some members of the taxa mentioned radically different

compounds replace aucubinlike glycosides. *Gentianaceae* produce gentiopirrin, swertiamarin and gentianin. The same is true for one tribe of *Loganiaceae*. *Oleaceae* accumulate oleuropein and many *Loganiaceae*, *Apocynaceae* and *Rubiaceae* synthesize the so called complex indolic alkaloids. Some members of *Apocynaceae*, *Bignoniaceae* and *Valerianaceae* are known to contain

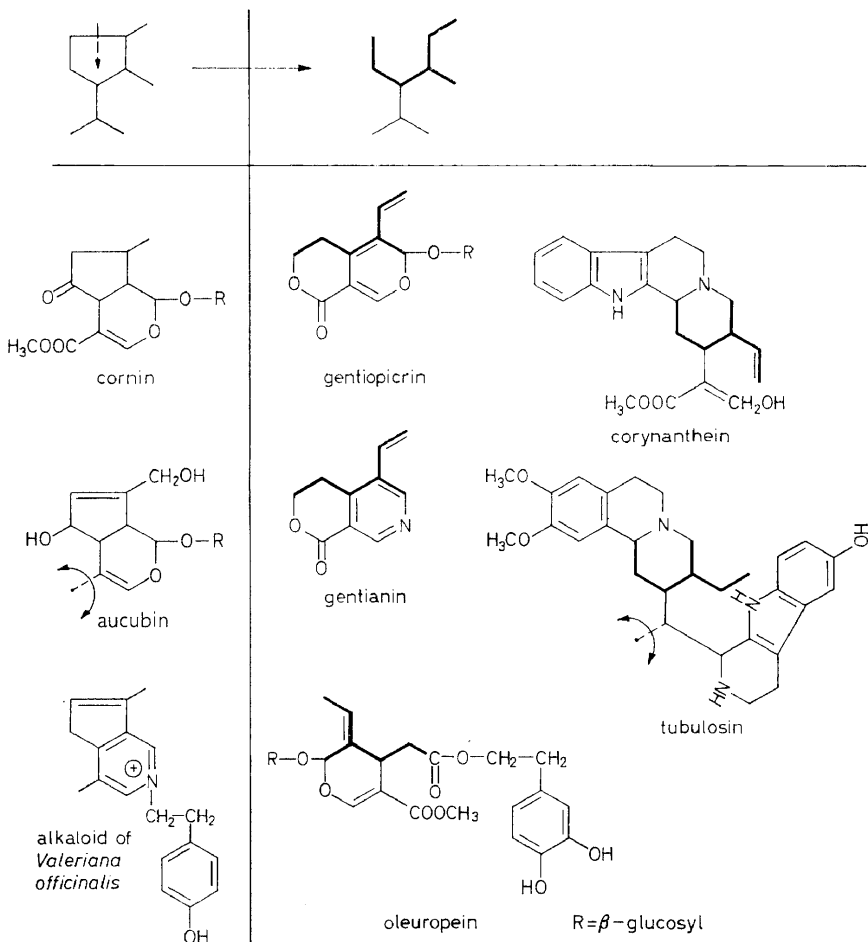


Figure 1. The homologous series of monoterpene iridoid, phytoconstituents

skytanthin-like alkaloids. An overwhelming number of chemically unlike constituents (cf. Figure 1) has been detected in the taxa mentioned. All these compounds, however, according to a hypothesis of Thomas³⁴ could arise along biogenetically very similar lines. Their molecules would represent partly (indolic alkaloids) or wholly (skytanthin-like alkaloids, gentianin, iridoid compounds) modified cyclopentanoid monoterpenes. Results of most recent investigations about the biosynthesis of different members of this assembly of phytoconstituents tend to confirm the hypothesis of Thomas.

CHEMICAL CHARACTERS IN PLANT TAXONOMY

If this is the truth, the whole group of compounds represents a homologous series because the different members of the group are elaborated along essentially similar lines. Notwithstanding pronounced chemical dissimilarities of members of a homologous series of chemical compounds the latter may indicate true relationship of plants accumulating them. On the other hand if within a sharply defined genus such as *Pinus*, some members (e.g. *Pinus sabiniana* Dougl. and *Pinus jeffreyi* Balfour) produce predominantly *n*-hexane and pinidin as volatile constituents of their leaves instead of the usual monoterpenes, this represents a case of true divergence. The deviating compounds arise from another pathway. Like true convergence, true divergence may be a factor rendering very difficult the elaboration of a natural system of plants. Like parallelism, chemical diversification may originate in different manners and its bearing on taxonomic problems can only be evaluated after a far-reaching analysis of the underlying facts.

The following discussion will be devoted to parallelism only. Moreover, for convenience, three types of convergent evolution will be discerned.

Parallel overall evolutionary trends in phylogenetically remote taxa

Biologically governed tendencies of flower and inflorescence evolution are rather well understood. Zygomorphic flowers or pseudanthia (a pseudanthium is a showy inflorescence imitating a single flower; all composites, e.g., bear pseudanthia) evolved independently in many insect-pollinated plant groups and inconspicuous, unisexual or protogynous flowers often aggregated in spiklet- or catkin-like inflorescences evolved in plants which reverted to wind pollination. Nobody classifies, e.g., all pseudanthia-bearing plants together because the individual flowers in pseudanthia usually preserve their characters and because some aspects of flower and inflorescence evolution resulting in many types of parallelism are rather well understood. For metabolic patterns and individual categories of constituents of angiosperms general tendencies of evolution are scarcely known at present. Alkaloids, for instance, have been detected in Fungi, Pteridophyta, Gymnospermae and Angiospermae but it is virtually impossible to indicate evolutionary trends concerning their structure and distribution. Within taxa of lower rank like species in a genus, genera in a family and even families in an order such tendencies may emerge in the near future but with regard to the whole plant kingdom such tendencies seem not to exist at all or are still far from being conceived clearly. Many instances of parallelism (e.g. distribution of senecionin-type pyrrolizidin alkaloids; distribution of aporphine-type alkaloids; distribution of tropan-type alkaloids) are known with regard to alkaloids but they are not yet understood in a satisfactory manner.

In other fields of plant chemistry the first indications for overall evolutionary trends begin to become apparent. Bate-Smith³⁵ and Lebreton³⁶ have put forward the hypothesis that in angiosperms, plants accumulating leucoanthocyanins and trihydroxylated phenols (leucodelphinidin, myricetin, gallic and ellagic acids) in leaves preceded plants not producing such compounds and that flavonol synthesis preceded the production of other types of anthoxanthins. If such general tendencies for the evolution of

phenolic patterns of leaves do indeed exist in angiosperms, many cases of chemical convergence (*e.g.* accumulation of apigenin and luteolin in non-related plant groups) become easily understandable.

Other examples of rapidly accumulating evidence for general evolutionary trends for plant metabolites may be found in the fields of the chemistry of lignin, hemicelluloses and cuticles and their waxes³⁷ and perhaps even in the field of triterpene chemistry³⁸.

An insight in general evolutionary trends for categories of plant constituents (*i.e.* knowledge of their "Merkmalsphylogenie") is taxonomically important in other respects too. Taxa possessing many progressive characters can be derived from taxa with characters of a lower evolutionary level but the reverse, of course, is impossible.

Parallelism arisen in connection with adaptation to environment

Many morphological and anatomical characters of plants are intimately connected with adaptations to special exigences of habitats. This immediately explains many cases of parallelism (and diversification) and prevents us from overrating the taxonomic implications of clearly adaptive characters.

Most probably the accumulation of many of the highly curious secondary plant metabolites as well as distinct patterns of regular plant constituents are the result of selection by environment. It would not seem surprising that a metabolic variant perfectly adapted to fixed conditions of plant life originated more than once in phylogenetically non-related taxa. But to understand and interpret the facts correctly, it is essential to know something about the ecological and biological meaning of chemical patterns of plants. With regard to the majority of the so-called secondary plant constituents our knowledge in this field is extremely poor. Fraenkel³⁹ has gone so far as to declare that "these odd chemicals arose as a means of protecting plants from insects and now guide insects to food". This, of course, can be only part of the story. Climatic and edaphic factors of plant habitats are not less important as selecting agents than are insects. Their influence on phytochemical patterns, however, is scarcely known. Hillis⁴⁰ obtained indications that in eucalypts stilbene production is correlated with the aridity of habitats and it seems that in essential oil bearing plants many of the intraspecific chemotypes represent probably populations selected predominantly by microclimates. It has been suggested that the flavonoid persicarin occurs essentially in marsh plants⁴¹ and if this proves to be true the compound may in some way be involved in hygrophilic adaptation. Secondary plant constituents moreover may help some species in their competition with other plants for a given habitat. It must, however, be agreed that we are still unaware of the true contribution of secondary plant metabolites to the overall fitness for life of plants.

In the field of ordinary plant metabolites our present-day position is perhaps a little better.

Carbohydrate accumulation in storage organs of perennial plants is a common feature. In chlorophytes, bryophytes, pteridophytes, gymnosperms and angiosperms sucrose and starch generally fulfil a storage function. There exist, however, many groups of plants which have largely replaced sucrose and starch by other carbohydrates. It is highly probable that such replace-

CHEMICAL CHARACTERS IN PLANT TAXONOMY

ments represent examples of progressive evolution correlated in some way with ecological features, e.g., with the colonization of less favourable habitats. Many rhizomatous species of *Iris* replaced starch partially or totally by irisin-type fructanes as they moved farther away from the Mediterranean centre of the genus. The Eurasiatic *Iris pseudacorus* L. and the Northern American *Iris virginica* L. and *Iris versicolor* L. store exclusively fructanes in their rhizomes. Similarly many of our perennial grasses are known to store fructanes in their rootstocks whereas tropical grasses seem to

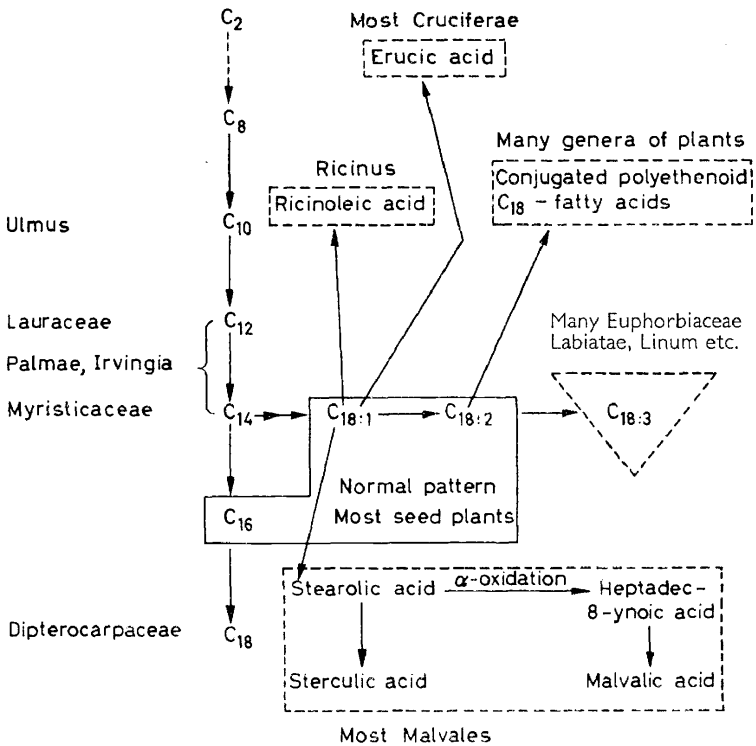


Figure 2. Possible derivation of some characteristic seed oils of plants from the most common pattern⁴⁴⁻⁴⁸.

accumulate sucrose and starch preferentially. The storage sugars of our perennial *Labiatae* are stachyose and higher oligogalactosides of sucrose while some tropical members of the family have retained starch accumulation. In the subfamily *Silenoideae* of *Caryophyllaceae* starch is replaced by oligogalactosides formerly called lactosin and presently known as belonging to the lychnose and isolychnose group of oligosaccharides.

Fatty oil is the main storage product in the seeds of many flowering plants. Triglycerides containing palmitic, oleic and linoleic acids as main fatty acids are by far the most common ones. However, in the field of seed oils too many deviations from this common pattern are known (cf. Hilditch⁴²; Shoreland⁴³). Such aberrant seed oils may be looked upon as specializations,

i.e. as the result of a process of progressive evolution, which, in many instances, may have been governed by external factors. Recent observations and speculations suggest that most of the "unusual" fatty acids encountered in seed oils arise from oleic or linoleic acid, *i.e.* by the addition of new steps to the ordinary pathway of fatty acid synthesis in seeds. Other "unusual" seed oils may be derived from the "usual" ones by suppression of a few of the ordinary steps. Some of the suggested connections are illustrated in *Figure 2*, which is based on the scheme of James *et al.*⁴⁴.

Several facts seem indeed to indicate that "unusual" seed oils originated in connection with ecological specialization. The predominantly tropical *Capparidaceae* produce seed oils of the normal type; the closely related extratropical *Cruciferae* have erucic acid as a main fatty acid in the seed oils of many of their members. Many *Labiatae* produce seed oils, rich in linolenic acid, while most of their tropical relatives seem to have oils of the ordinary type. In the genus *Cucurbita* trichosanic acid seems to be restricted to the specialized and genetically and geographically isolated xerophytic species *Cucurbita digitata* Gray, *C. palmata* Wats. and *C. foetidissima* H.B. et K. In this respect it is interesting to note that Rehm⁴⁹ reported that seedlings of the more advanced species of *Cucurbita* contain cucurbitacin E whereas seedlings of the more primitive species contain cucurbitacin B only. He investigated *Cucurbita palmata* and *C. foetidissima*, too; in seedlings of both species cucurbitacin E is present.

Distinct types of specialization are likely to have occurred in several non-related taxa. The more a special chemical character is connected with adaptation the more the incidence of parallelism is to be expected. If, for instance, we accept for the evolution of seed oils the progression oleic—→ linoleic—→ linolenic acid and if at the same time we are able to demonstrate clearly an advantage of the linolenic type in a cold climate then the fact that seed oils rich in linolenic acid are characteristic for several non-related taxa will no longer be an argument against the taxonomic potentialities of chemical characters.

Accidental Parallelism

Morphological parallelism seems to be purely accidental in many instances. It may solely be the result of an unlimited bias of nature for variation giving rise to a tremendous series of forms many of which may be neither profitable nor deleterious in the struggle for life and therefore will hardly be affected by selection through environment. One of the astonishing aspects of nature is its power to achieve a certain goal by a seemingly unlimited number of variants. Nature has been compared with a playing child⁵⁰ whose activities are not governed by economics and expediency but rather by imagination and by the pleasure in experimentation.

The number of non-related plants bearing similar leaves is very large. *Tropaeolum*, *Umbilicus* and *Hydrocotyle* or *Trifolium* and *Oxalis* may be cited as examples. Many types of chemical parallelism originate probably in a similar manner (*e.g.* isoflavones in *Podocarpus* and several families of angiosperms; bioflavonoids in *Coniferosida*, *Casuarinaceae* and *Caprifoliaceae*).

Limitations caused by incorrect identification and by the omission of documentation

Some of the preceding discussion should already have demonstrated that in many instances the correct identification of plant samples is a far from easy task. To sum up some factors causing difficulties and ambiguities the following ones very often may be involved.

1. Many species of plants are complex aggregates, their members being often characterized predominantly cytologically or ecologically. Their taxonomic treatment may change with time and may moreover be dependent on the systematists' personalities working at a given time with the aggregate. Taxonomy and nomenclature very often become highly troublesome and disappointing in such entities.

2. In many aggregate species and in many genera with taxonomically good but morphologically rather concealed species a correct identification implies a rather intimate acquaintance with the plants concerned.

3. Hybrid origin of plant samples may often cause difficulties of identification. Conditions for hybridization are especially favourable in Botanical Gardens where many species are grown close together.

4. Many floras of the world, especially those of tropical countries are still poorly known and only superficially studied from a taxonomic point of view. Every modern revision results in a large number of reductions of species and sometimes even genera. Recombinations and descriptions of new taxa are moreover considered necessary by every taxonomist revising a group of tropical plants or monographing a tropical genus or family.

The facts mentioned and many others imply that in many instances the result of plant identification depends on the paper or the flora used for this purpose. Even if a taxonomist is consulted for help with plant identification the name given to the plant material will be dependent on his acquaintance with and his personal interpretation of the respective group of plants.

There is only one means of escaping all ambiguities in the matter of plant identification. It consists in documentation. Each scientist working with plant material should understand and accept the obligation to document botanically his plant sources. This implies that perfect herbarium specimens are prepared and adequately (time and locality of collection) labelled. The specimens should be deposited in a herbarium accessible to other scientists. The specimen numbers and the institution where specimens were deposited should always be given in phytochemical publications. If herbarium specimens cannot be prepared because crude drugs (woods, seeds, commercial crude drugs) are investigated it should never be forgotten to preserve an adequately labelled representative sample of this material and to deposit it in a crude drug collection accessible to other scientists. To illustrate the importance of such a procedure I should like to give a recent example. Indian workers⁵¹ isolated a series of coumarins from roots of *Nardostachys jatamansi* DC. (*Valerianaceae*) commercially available. These coumarins seemed out of place to me in *Valerianaceae*. Professor Bhattacharyya (of National Chemical Laboratory, Poona, India) was kind enough to send me a sample of the crude drug investigated. The anatomy of the roots indicated

clearly that the crude drug did not represent the rootstock of *Nardostachys jatamansi* but of an umbelliferous substitute.

An adequate documentation of the starting material of each phytochemical investigation is the only means of minimizing the consequences of the very frequent errors in plant identification, because documentation makes possible rechecking determinations at any given time. Phytochemical literature is full of errors of plant identification and plant naming. To prevent continuation of this undesirable situation every chemist and botanist working with plants should undertake the necessary steps, troublesome as they may be, to guarantee an adequate documentation of his starting materials. If one realizes that systematic botany is even more interested in the results of phytochemical research than chemistry, which can study its problems with pure synthetics as well, one will immediately perceive that the troubles involved in an adequate documentation will be recompensed by imparting a more general scientific value to the results of the investigations.

Greshoff⁵² addressed the following words to an audience of scientists in 1890 "Wellicht gelukt het later deze hypothese (i.e. that chemical characters are valuable for taxonomic botany) meer zekerheid te geven, en komt de tijd dat de chemie op haar beurt aan de botanie een deel der goede diensten terugbetaalt, die deze wetenschap nu aan haar bewijst"[†]. This period has now been reached without doubt. But phytochemistry must observe a meticulous documentation if she really intends to repay systematic botany part of the support which the latter science has always offered to her.

References

- ¹ A. P. DeCandolle. *Essai sur les propriétés médicales des plantes, comparées avec leurs formes extérieures et leur classification naturelle*, first edition, Paris (1804); second edition, Paris (1816).
- ² M. Greshoff. *Ber. Deut. Pharm. Ges.* **3**, 191 (1893).
- ³ F. Rochleder. cf. e.g. *Ann. Chem. Pharm.* **83**, 64 (1852).
- ⁴ M. Greshoff. Mededeelingen uit 's Lands Plantentuin No. VII (Batavia 1890) and No. XXV (Batavia 1898).
- ⁵ L. Rosenthaler. *Beih. Botan. Zentralbl.*, 1. Abt. **21**, 304 (1907).
- ⁶ R. T. Baker, and H. G. Smith. *A Research on the Eucalypts and their essential oils*, second edition, Government Printer, Sydney (1920).
- ⁷ M. Wheldale. *Biochem. J.* **5**, 445 (1911).
- ⁸ S. Iwanow. *Beih. Botan. Zentralbl.*, 1. Abt. **32**, 66 (1915); *Ber. Deut. Botan. Ges.* **44**, 31 (1926).
- ⁹ H. Colin. *Rev. Gen. Sci. Pures et Appl.* **46**, 165 (1935).
- ¹⁰ H. Molisch. *Pflanzenchemie und Pflanzenverwandtschaften*, G. Fischer, Jena (1933).
- ¹¹ J. B. McNair. *Studies in plant chemistry including chemical taxonomy, ontogeny, phylogeny, etc.* (A collection in book form of papers of the author between 1916 and 1945). Published by the author, Los Angeles, California (1965).
- ¹² Th. Weevers. *Rec. Trav. Botan. Néerl.* **30**, 336 (1933); *Koninkl. Akad. Wetensch. Amsterdam, Proceedings* **39**, 757 (1936); *Blumea* **5**, 412 (1943).
- ¹³ M. Bridel, and A. Kramer. *Compt. Rend.* **193**, 748 (1931).
- ¹⁴ R. Wettstein. *Handbuch der systematischen Botanik*, 4. Aufl., F. Deuticke, Leipzig und Wien (1935).
- ¹⁵ A. A. Pulle. *Compendium van de terminologie, nomenclatuur en systematiek der zaadplanten*, third edition, N.V.A. Oosthoeks Uitg. Mij., Utrecht (1952).

† Perhaps it will be possible at a later date to judge better the taxonomic meaning of chemical characters and the time may arrive when chemistry will be able to render to botany part of the help the latter has always offered to phytochemistry.

CHEMICAL CHARACTERS IN PLANT TAXONOMY

- ¹⁶ A. Cronquist. *Bull. Jardin Botan. Bruxelles* **27**, 13 (1955).
- ¹⁷ J. Hutchinson. *The Families of flowering plants*, second edition, Clarendon Press, Oxford (1959).
- ¹⁸ A. Takhtajan. *Die Evolution der Angiospermen*, G. Fischer, Jena (1959).
- ¹⁹ A. Engler. *Syllabus der Pflanzenfamilien*, 12. Aufl., Band 2, Gebr. Bornträger, Berlin (1964).
- ²⁰ R. F. Thorne. *The American Naturalist* **97**, 298 (1963).
- ²¹ L. Benson. *Plant taxonomy. Methods and principles*. The Ronald Press Comp., New York (1962).
- ²² P. H. Davis, and V. H. Heywood. *Principles of Angiosperm taxonomy*, Oliver and Boyd, Edinburgh-London (1963).
- ²³ H. Solereder. *Systematic anatomy of the Dicotyledons*, Clarendon Press, Oxford (1908).
- ²⁴ C. R. Metcalfe, and L. Chalk. *Anatomy of the Dicotyledons*, Clarendon Press, Oxford (1950).
- ²⁵ S. Carlquist. *Comparative plant anatomy*, Holt, Rinehart and Winston, New York (1962).
- ²⁶ P. Maheshwari. *An introduction to the embryology of Angiosperms*, McGraw-Hill Book Co., New York-Toronto-London (1950).
- ²⁷ R. P. Wodehouse. *Pollen Grains*, Hafner Publish. Co., New York (1959).
- ²⁸ G. Erdtman. *Pollen morphology and plant taxonomy. Angiosperms*. The Chronica Botanica, Waltham, Mass. (1952).
- ²⁹ C. D. Darlington. *Chromosome botany and the origins of cultivated plants*, second edition, George Allen and Unwin Ltd., London (1963).
- ³⁰ I. Manton. *Problems of cytology and evolution in the Pteridophyta*, University Press, Cambridge (1950).
- ³¹ R. Hegnauer. Chemismus und systematische Stellung der Cornaceae, in *Festschrift Kurt Mothes zum 65. Geburtstag*, p. 235-246, G. Fischer, Jena (1965).
- ³² R. Hegnauer. *Chemotaxonomie der Pflanzen*, Vol. 3, p. 565-569 and fig. 29 on p. 544, Birkhäuser, Basel (1964).
- ³³ D. B. O. Savile. *Science* **120**, 583 (1954).
- ³⁴ R. Thomas. *Tetrahedron Letters* 544 (1961).
- ³⁵ E. C. Bate-Smith. *J. Linn. Soc. London, Botany* **58**, 371 (1962).
- ³⁶ Ph. Lebreton. *Bull. Soc. Botan. France* **111**, 80 (1964).
- ³⁷ Cf. R. Hegnauer, *Chemotaxonomie der Pflanzen*, Band 1, p. 192-219 and 307-310, Birkhäuser, Basel, 1962; E. A. Baker and J. T. Martin, *Nature* **199**, 1268 (1963); A. M. Silva Fernandes, E. A. Baker, and J. T. Martin, *Ann. Appl. Biol.* **53**, 43 (1964); T. E. Timell. *Svensk Papperstidning* **65**, 266 (1962).
- ³⁸ R. Hegnauer. *Lloydia* **23**, 267 (1965).
- ³⁹ G. S. Fraenkel. *Science* **129**, 1466 (1959).
- ⁴⁰ W. E. Hillis, and K. Isoi. *Phytochemistry* **4**, 541 (1965).
- ⁴¹ H. Tatsuta, and Y. Ochii. *Sci. Reports Tohoku Univ.*, First series **39**, 236 (1956).
- ⁴² T. P. Hilditch, and P. N. Williams. *The chemical constitution of natural fats*, fourth edition, Chapman-Hall, London (1964).
- ⁴³ F. B. Shoreland. The distribution of fatty acids in plant lipids, in T. Swain. *Chemical plant taxonomy*, p. 253-303, Academic Press, London-New York (1963).
- ⁴⁴ A. T. James, R. V. Harris, C. Hitchcock, B. J. B. Wood, and B. W. Nichols, *Fette, Seifen, Anstrichmittel* **67**, 393 (1965).
- ⁴⁵ G. N. Smith, and J. D. Bu'Lock. *Chem. and Ind.* 1840 (1965).
- ⁴⁶ F. D. Gustone. *Chem. and Ind.* 1033 (1965).
- ⁴⁷ D. T. Canvin. *Canad. J. Botany* **43**, 49, 63, 71 (1965).
- ⁴⁸ Z. B. Kondra, and B. R. Stefansson. *Canad. J. Genetics Cytol.* **7**, 500 (1965).
- ⁴⁹ S. Rehm. *Ergebnisse der Biologie* **22**, 108 (1960).
- ⁵⁰ K. Mothes. *Naturwissenschaften* **52**, 571 (1965).
- ⁵¹ S. N. Shanbhag, C. K. Mesta, M. L. Maheshwari, S. K. Paknikar, and S. C. Bhattacharyya. *Tetrahedron* **20**, 2605 (1964); **21**, 3591 (1965).
- ⁵² M. Greshoff. *Planten en plantenstoffen*; lecture held on 11 December 1890 in Batavia; published by Koninklijke Natuurkundige Vereniging in Nederlands-Indië, (voordrachten No. 7), Ernst and Co., Batavia and Noordwijk (1891).