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II. ON "NUMERICAL CHEMOTAXONOMY" REVISITED

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For those of us who are active in numerical taxonomy using chemical data (often called numerical-chemotaxonomy), the article by Weimarck (1972) seems a voice from the past. The same questions have been raised (see Adams, 1970; Adams & Turner, 1970; Adams, 1972a; Adams, 1972b; Flake, von Rudloff & Turner, 1969) in several ways. The papers cited by Weimarck as being examples of the poor use of chemical data (under 4(a)) were published in 1962, 1964, 1965, 1967, 1967, 1968, 1968, and 1969. The research for those works was accomplished before 1968. Five years ago!

It appears that Weimarck lends some special category to chemical characters since he states "Spot patterns of nonidentified substances on chromatograms are certainly not very suitable characteristics for numerical evaluation of differences between taxa." Although I agree that this data is generally of less significance than when the compounds have been identified, the question could also be raised concerning morphological characters since in most instances their mode of inheritance is not known nor their function, much less the morphogenetic path! The question of different biosynthetic paths for camphor in different taxa is fundamentally no different than the question of homology of trichomes in different families.

The problem of choosing a similarity measure such that one's hypothesis is upheld is certainly a valid criticism but one wonders how many morphological characters have been discarded because "characters that are likely to give the *wrong* picture must be eliminated" (Italics mine), according to Wagner (1969, p. 74)? By a prejudicial choice of morphological characters (either consciously or sub-consciously) one can easily arrive at a classification which supports your hypothesis. The pitfalls of various similarity measures and clustering methods are well documented and most systematists are well aware of these problems (although I do admit that there are unfortunately many systematists who are misusing "canned" numerical

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programs). From my survey of the literature, I would say that chemosystematists and the more classical systematists are about equally guilty.

As for the "subjective" evaluation of data by computer processing, it should be noted that subjectiveness enters in the human choice of which programs to use and not in the actual computer processing. In the final analysis, the worth of a study is only as good as the strength of the biological question asked and the logical method (algorithms) used in the evaluation (numerical treatment) of the data.

I applaud Weimarck for his insistence on the use of more than one specimen to represent a taxon. In all fairness though one must admit that in many of the works cited, infraspecific variation was thought to be very small for biochemical characters. It is only in the past five years that good populational studies have been made which have shown chemical characters to be very similar to morphological characters in populational variability, seasonal variation, and ontogenetical variation (much to the naivety and chagrin of the organic chemists-turned-systematists).

Weimarck criticizes the use of numerical methods to identify two taxa which share 40 compounds and differ in the 41st. compound. Surely few systematists today would compute similarity measures to attempt to distinguish between these taxa. The use of computer techniques are really most useful when one is trying to quantify differences between several taxa considered simultaneously. The case cited is very similar to that cited by Runemark (1968) in the use of numerical taxonomy to detect hybridization. It should be obvious to most that even when complete complementation occurs in all the chemical characters, simple matching coefficients are not suited to show exact ancestorial relationships. For instance, in the example by Runemark (1968), species A contained spots 1-20 and species B contained spots 21-30, the hybrid contained all spots, 1-30. Thus, a simple matching coefficient would show the hybrid to be more closely related to species A ($Sr_{A\text{-}hybrid} = .67$, $Sr_{B\text{-}hybrid} = .33$). Immediately many people are upset because the hybrid is not intermediate between the parents. This shows our morphological bias! Chemical compounds have been documented to generally be complementary in the hybrids, not intermediate as in the case of many morphological characters. I agree that new numerical methods are needed to express chemical evidence of hybridization.

In examination of Weimarck's work on chemical leaf constituents (1970), I am reminded of my work in *Juniperus*, where I have carefully examined populational variation, seasonal variation and ontogenetic variation in several species in the southwestern United States. Yet in my current research on the Junipers of Mexico, I had to rely on these studies for evidence concerning the best sampling period, how to sample, and even sampling density. The support and scope of the problem prohibits detailed population sampling from many areas within each taxa (22 taxa in Mexico), in addition it would take years to obtain detailed results on seasonal variation in the terpenoids for each taxon as has been done in *Juniperus scopulorum* (Powell and Adams, 1973).

Another factor to be considered is the purpose of a study. In the Junipers of Mexico I am particularly interested in the taxonomy and phylogeny of these taxa versus others in North America. Experience has shown that comparisons between species tolerates much coarser data than comparisons between populations within a species. Certainly in order to avoid a lifelong project for each taxon, we must rely on information gathered on

other related species. Perhaps I should note that I have not said that detailed population, ontogenetic and seasonal variation studies are not necessary. Detailed populational, genetical, and seasonal variational studies will undoubtedly lay the concepted framework for chemical data just as such studies have done for morphological characters.

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