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Editorial

Guidelines for consistent characterisation and documentation of plant source materials for studies in phytochemistry and phytopharmacology

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A B S T R A C T

Plants are still by far the most important source of natural products. For higher plants as source materials identification and documentation are less challenging than for many other groups of organisms such as microorganisms or marine invertebrates. Nonetheless, many studies in natural products chemistry and phytopharmacology involving higher plants are flawed because the plant material is erroneously assigned, inaccurately documented, untraceable, or not named in accordance with the rules of nomenclature. Recently, the importance of the proper usage of plant nomenclature has been highlighted in a dedicated series of articles in the *Journal of Ethnopharmacology* and the importance of taxonomic and geographic information in a viewpoint in *Natural Products Reports*. Here, the importance of three related points is being emphasized: a) the traceability of the identification of plant source materials, b) easy access to vouchers and digital vouchers of the studied plants, and c) standards for accurate geographic data about the collection sites of these plants.

1. Introduction

In any investigation of plant material, correct identification is a prerequisite for meaningful phytochemical and phytopharmacological studies. In analogy, this of course holds true for all studies in natural products chemistry and their respective source taxa. However, in the present discussion, the focus will be on higher plants. Though explicitly or implicitly acknowledged as important in all relevant guidelines, currently little attention is often paid to correct plant identification and the documentation of this identification by authors and editors of phytochemical research papers. Proper plant identification, especially for plants collected in the wild, is a complex and underestimated task requiring expertise and experience. This holds particularly true for regions with a high biodiversity but little or no tradition in systematic botany. With the current and recently often lamented decline in taxonomic training (Kholia and Fraser-Jenkins, 2011; Heinrich and Verpoorte, 2014; Leal et al., 2016), the problems related to correct plant identification within applied plant sciences such as phytochemistry and ethnobotany become more and more pressing. On the other hand, modern technologies give unprecedented possibilities for making taxonomic samples available in a fast and cost efficient manner. First, DNA barcoding initiatives can support or contradict plant identifications made on purely morphological grounds (Chen et al., 2010). Secondly, the opportunities to determine precisely the collection site(s) of plant samples have dramatically improved in the last decades, a capacity still seldom yet used to the benefit of their manuscripts by many phytochemists. The exact location of collection sites as a requirement for reproducible studies in applied plant sciences is mentioned here in the context of plant determinations because, even when plant taxa are correctly assigned, sometimes pronounced geographical variation may show significant disparity in plant specialised metabolites patterns (Bohm, 2009). Thus, the same plant taxon might or might not, depending on the origin of the plant material, constitute or not constitute an adequate source for particular natural products.

With these points in mind, the aims of this communication are:

1) promoting the usage of taxonyms instead of mere scientific names to make plant identifications traceable,
2) promoting digital vouchers as a means to document plant determination results,
3) promoting a standardised accurate georeferencing of plant collection sites to make reduplications of phytochemical studies feasible.

To this end, amendments to the guidelines (and editorial practices) of relevant journals such as *Biochemical Systematics and Ecology, Fitoterapia, Journal of Natural Products, Phytochemistry*, and *Phytochemistry Letters* as well as related journals are proposed. Examples to highlight the problem from all listed journals are abundant (including previous publications by the author himself) but are omitted here in order not to give the false impression of intending to criticise personally the authors of articles and/or the editors of journals used as examples.

However, I am convinced that changes in authorial and editorial

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practices are needed and that these should be consistently implemented as soon as possible.

2. Useful conventions in systematic botany

Phytochemists, ethnobotanists, ethnopharmacologists, and scientists in many other fields of applied plant science rely on, but do not actually study, plant biodiversity. Unfortunately, not all of these scientists are aware of the problems involved in correctly identifying plant taxa and of the importance of precisely documenting the geographical origin of plant samples, a situation recently discussed by Leal et al. (2016). In fact, some papers imply that merely naming the source species will enable interested readers to repeat the described experiments, thus, treating plant samples in the same way as other commodities, such as commercially-available biochemicals. However, in applied plant science this approach is not tenable because correct plant identification is a complex process that does not always lead to unambiguous results. The following are some of the principle factors to be considered in this context:

1. Expertise of the person(s) identifying the plant samples.
2. Biodiversity of the area in which the plants were collected.
3. Quality of reference works for plant identification for the region in which the plants were collected.
4. Existence of closely related and/or morphologically similar taxa in the region in which the plants were collected.
5. Existence and access to herbaria with vouchers for comparison and access to experts to verify the identification results.

Even if identification is performed by experts, the nomenclature of plants collected in the wild cannot always be determined without a degree of uncertainty. Botanists employ a set of terms specifically designed to highlight this fact (Stearn, 1996; Mabberley, 2008):

aff. (or *sp. aff.* or *affin.*) *species affinis* indicates that the investigated material is related to, has an affinity to, but is not identical to, the species with the binomial name that follows. This abbreviation might also indicate that the material belongs to a new, yet undescribed species.

agg. stands for 'aggregate' or 'species complex' and is indicated after the binomial name. This abbreviation is used to indicate that the material belongs to the species complex but not, or not necessarily, to the micro-species bearing this name. The abbreviation agg. is most often used for species complexes containing numerous hard to differentiate micro-species, e.g. in groups where apomixis and polyploidy occur such as *Rubus* and *Taraxacum*.

cf. (for *confer*) means literally "compare with" is used in front of a taxon name and indicates that the identification is uncertain.

s.l. is the abbreviation for *sensu lato*, i.e. in the wide or broad sense. This abbreviation is used in situations when the taxon name it follows is used in different meanings in the scientific literature and the broader application of this name instead of the narrower application (s.str. *sensu stricto*) is intended.

sp. (or *spp.* for the plural) indicates that the material belongs to the genus mentioned in front of the abbreviation without indicating a species, without indicating possible affinities but sometimes implying that the material belongs to a potentially new species. Identification has thus either not yet been completed or the available evidence is insufficient to assign the specimens to a known taxon.

Unfortunately, these helpful identifiers are only very rarely used in phytochemical and phytopharmacological research papers (positive exceptions are e.g. Martínez-Vázquez et al., 1990; Dellar et al., 1994; Gibbons et al., 1997). In systematic botany, the absence of these identifiers implies that the voucher/plant was identified unambiguously; in the applied plant sciences it unfortunately often only means that the authors were not aware of the existence of these identifiers or of the potential ambiguity of the obtained identification results.

3. Problems related to systematic botany with existing guidelines of journals in the field of phytochemistry and their application in phytochemical research papers

The main focus of this "Editorial" is not *per se* the actual correctness of the identification of the plant material (though this of course is crucial) but rather to discuss the accessibility of the information related to plant collection (where exactly were the plants collected), identification (how were the plants identified, i.e. which flora/characters were used), naming (how is the used scientific name defined, i.e. which is the taxonym), and the physical and digital evidence documenting this information (voucher specimens and scans/pictures of these voucher specimens). This information is crucial, because even studies on wrongly assigned plant material can be valuable sources of information for follow up studies if enough information is provided to reproduce the described studies. At the same time, it also can lead to the eventual correction of the erroneous plant identification [for an example from my own studies please refer to Zidorn et al. (2004), Samuel et al. (2006), and Zidorn et al. (2007)].

At first glance, the author guidelines of relevant journals such as *Biochemical Systematics and Ecology*, *Fitoterapia*, *Journal of Natural Products*, *Phytochemistry*, and *Phytochemistry Letters* fulfil the criteria to indicate the taxonomy and provenience of the collected material. However, in a survey of recent (2013–2015) original papers in the five journals mentioned above dealing with natural product isolation from non-cultivated plants, the following observations were made:

1) Voucher specimens and their respective numbers and the herbaria they are deposited in are often, but not always, indicated. Likewise, the herbarium code (such as K for Kew Gardens) is often, but not always, stated. A common problem is related to referrals to Departmental Herbaria, which might not participate in inter-institutional voucher loans. Thus, vouchers deposited in these herbaria might not be available to phytochemists for verification of plant determinations.
2) Scans or pictures of voucher specimens (digital vouchers), though of extremely high value to check morphologically based plant identifications, are regularly missing and providing them is not actively encouraged by current editorial practices.
3) Scientists identifying the plants are often named, while the literature employed for plant determination, though essential to know in which definition/delimitation scientific plant names were understood (taxonym), is only rarely cited.
4) Uncertainties of plant identifications are suspiciously rarely stated (see also explanations in section 2.). These are – even for experts – not uncommon in critical groups, although they might be irrelevant for the chemical parts of publications. Therefore, it is to be assumed that many plant identifications for phytochemical studies appear to be more specific, secure, or unambiguous than they really are. Though actually irrelevant for the reported chemistry, this might prove fatal for (chemo-) systematic studies based on such papers. It becomes of crucial importance, however for comparing phytochemical