World Patent Information 34 (2012) 206–212

Contents lists available at SciVerse ScienceDirect

World Patent Information

journal homepage: www.elsevier.com/locate/worpatin

Best practice in search and analysis of chemical formulations: From chemical recipes to complex formulation types and dosage forms☆

Maik Annies*

Syngenta International AG, Schwarzwaldallee 215, CH-4058 Basel, Switzerland

Keywords:
Chemical formulations
Formulation recipe
Formulation type
Dosage form
Non-patent literature
Prior art
Freedom-to-operate
Patentability
Novelty
Validity
E-journals
Chemical structure searching
Internet
Meta-search engines
Chemical identifier
InChI

A B S T R A C T

Chemical formulations are compositions of active ingredients and inert formulation components (adjuvants), which are more effective in combination than the active ingredients alone. Thus, formulation technology synergistically can improve the properties of active ingredients with regards to various aspects like application, uptake, safety or storage. Chemical formulations have a broad scope of uses ranging from pharmaceuticals and agrochemicals to cosmetics and materials protection. Since they represent the product as it is finally brought to market they have a high commercial and patent value.

Comprehensive search and retrieval of chemical formulations both in patent and non-patent literature builds the basis of a successful reinforcement of patent protection, avoidance of infringement of third party patent rights and competitive analysis. The paper discusses the various aspects of chemical formulations to be considered in chemical formulation searching, and presents best practice strategies for search, retrieval, and analysis of both patent and non-patent literature as well as internet content preferably related to agrochemical and pharmaceutical formulations.

1. Introduction

Active ingredients like pharmaceuticals, agrochemicals or cosmetics are normally not brought to market in their pure form but as formulations, i.e. in combination with inert formulation components (adjuvants). The purpose of these formulation components is to improve the properties of the active ingredient with regards to various aspects like biological effectiveness, application, uptake or storage. Since chemical formulations are the products as sold they have a high commercial value, and are well represented in chemical companies' product pipelines and portfolios. Efficient patent protection is therefore crucial to secure freedom-to-operate and avoid infringement and double inventions with regards to formulation technology. Formulation patenting also allows extending the patent lifecycle of active ingredients after patent protection of compounds *per se* and mixtures has expired and can thus expand freedom-to-operate and commercial effectiveness of newly developed compounds.

The business value of chemical formulations is also best reflected by the number of patent applications over the recent years. From 2000 to 2007 the number of priority filings related to chemical formulations (represented by the number of patent documents coded for chemical formulations in World Patents Index; see Fig. 1) continuously increased with slight decreases in 2008 and 2009, most probably caused by the worldwide financial crisis, which obviously had an effect on R&D expenditures and overall patent filing activities in various countries [1], and again in 2011.

As in other technology fields, search, retrieval and analysis of chemical formulations builds the basis of effective patenting strategies. Due to the complexity of the subject matter and the various aspects to be analysed it is therefore crucial to develop best practice search strategies for both patent and non-patent literature.

Chemical formulations are characterised by two major aspects to be considered in patent and non-patent literature searching: (a) the pure combinations of active ingredients and formulation components (the formulation recipe) and (b) the physical form of the chemical formulation as it is applied to their substrate (the formulation type or dosage form). The paper first exemplifies strategy design, search and retrieval for formulation recipes and formulation types/dosage forms published in patent literature, followed by specific issues arising from search and retrieval of

☆ Some of the subject matter of this article is based on a presentation of the author at the International Conference for the Information Community (ICIC) in October 2010 in Vienna, Austria.

* Tel.: +41 61 323 04 43.
E-mail address: maik.annies@syngenta.com.

0172-2190/$ – see front matter © 2012 Elsevier Ltd. All rights reserved.
doi:10.1016/j.wpi.2012.03.003

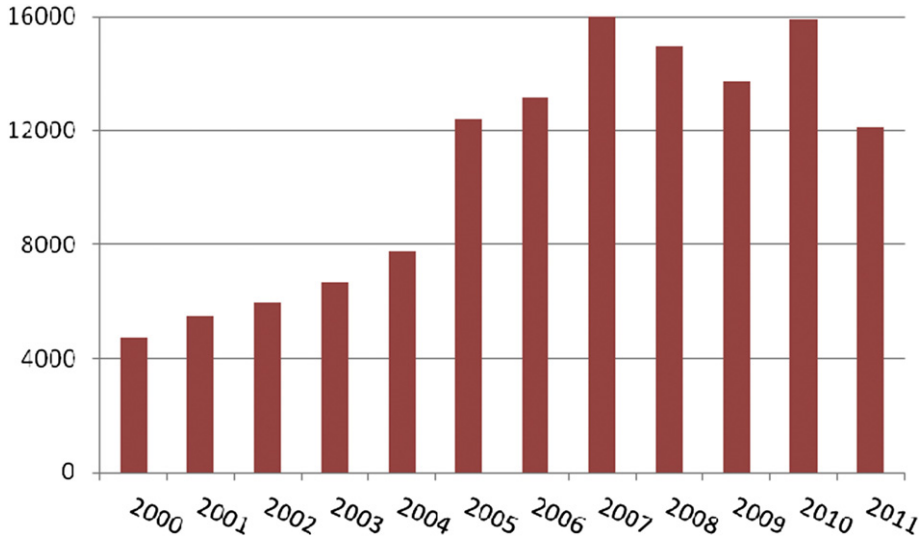

Fig. 1. Priority applications per publication year coded for both agrochemical and pharmaceutical formulations (Derwent Manual Codes C12-M and B12-M) in World Patents Index.

formulations in non-patent literature, including the internet. Finally, evaluation and analysis of documents related to chemical formulations in both patent- and non-patent literature will be discussed.

2. Chemical formulation searching in patent literature

2.1. Formulation recipes

Formulation recipes define the exact composition of active ingredients and inert formulation components as well as their concentration and proportions. The design of search strategies for formulation recipes critically depends on the type of search request. Typically, in patent literature formulation recipes are claimed in a fallback line from broad to specific, with broad generic classes of compounds disclosed in the first claim, which are narrowed down in the depending claims (see Fig. 2). As a consequence from a legal perspective, particularly in freedom-to-operate searching both specific and generic aspects of active ingredients and formulation components should be considered in patent literature, which comprises (a) the mixture of active ingredients (in case the formulation comprises more than one active ingredient), (b) the sub-mixtures of active ingredients with each of the formulation components, (c) each combination of formulation components among themselves (i.e. without active ingredients), and (d) broad general uses of the formulation components in chemical formulations.

Since formulations often contain numerous formulation components, particularly (c) and (d) can lead to complex search results with huge answer sets to be evaluated. However, many formulation components as well as their combinations are often used with only slight variations compared to already known or even commercialised formulations. To avoid doubling of efforts by searching known combinations repeatedly, it is therefore advisable to keep track of formulations already searched before or probably even sold. A precise documentation of previously searched formulation recipes and/or ideally in-house databases containing formulations already developed or sold are therefore a key factor for economic and time-saving formulation searching.

In contrast to freedom-to-operate searching, novelty and validity research related to chemical formulations encompass both patent and non-patent literature (for non-patent literature search and retrieval see Section 3). While novelty searches rather focus on the exact combination of active ingredient(s) with all formulation components as defined by the formulation recipe without taking into account sub-mixtures, validity searches should principally encompass the whole body of prior art including sub-mixtures as soon as they can be used to invalidate third party patents by proving a lack of inventiveness.

Specific search strategies for both active ingredients and formulation components should contain both CAS REGISTRY-numbers as well as common names, (IUPAC-) chemical names, lab codes and further synonyms taken from CAS REGISTRY or, free chemical databases like ChemSpider or ChemIDplus [2,3]. Trade names of active ingredients and formulation components are seldom used in patent literature and should, if at all, only be included if retrieval is not leading to unspecific search results from other subject areas not related to the chemical compounds of interest.

For generic retrieval especially important in freedom-to-operate searching of both active ingredients and formulation components, generic chemical names, database codes, controlled vocabulary and patent classifications for broad generic classes of chemical compounds should be taken into consideration if available. Substructure searching of both active ingredients and formulation components, e.g. in structure searchable databases like MARPAT, MMS (Merged Markush Service), CAS REGISTRY and WPIX (Derwent World Patents Index) can additionally improve search results.

Both specific and generic retrieval of formulation recipes may be further enhanced by searching full-text databases (e.g. PCTFULL, EPFULL, USPATFULL) useful in identifying hidden prior art not indexed by bibliographic databases (for identification of hidden prior art in non-patent literature see Section 3.1), e.g. in novelty and validity searching. In this context it is important to combine active ingredients and formulation components in full-text search strategies by appropriate proximity operators to keep control of retrieval and avoid large and rather unspecific answer sets.

A typical broad generic class of important and commonly used formulation components are polymers having various functions in improving the properties of active ingredients, e.g. as surfactants, dispersants or shells of microcapsules containing active ingredients. Polymers in formulations are often difficult to search with specific keywords or REGISTRY-numbers, since these strategies do not cover all generic aspects and structural variations (e.g. chain length, varying repeating units, monomer arrangements, tacticity)