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SPECIAL UNION FOR THE INTERNATIONAL PATENT CLASSIFICATION (IPC UNION)

COMMITTEE OF EXPERTS

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REQUEST FOR REVISION OF THE
INTERNATIONAL PATENT CLASSIFICATION (IPC)

Document prepared by the International Bureau

The Annex to this document contains a proposal for the creation of a new subclass on combinatorial chemistry made by the United Kingdom following a revision request submitted to the Committee of Experts (see document IPC/CE/29/7, Annex 1).

[Annex follows]

ANNEX/ANNEXE

C40B Combinatorial chemistry proposal

Please find attached detailed IPC revision proposal for C40B combinatorial chemistry. As discussed at the last meeting of the revision working group, the proposal only contains a very broad breakdown of main groups. I anticipate it will largely be necessary to classify elsewhere as well as in this subclass according to the actual chemical structures involved. I will attempt to define "line notes" (references to other areas of IPC) in due course.

Being a totally new subclass, I though it was a great opportunity to try our proposed new format for subclasses. I have therefore devised a very sparse subclass with allied classification definitions for the subclass and various main groups. It is my intention to hyperlink the various definitions to the relevant parts of the schedule to which they relate but I haven't actually made the links as I thought they would not translate to Word format.

I apologise that the details of this schedule have been submitted so long after the original notification of submission of a proposal. I'm sure you and all my colleagues in IPC will let me know what they think of a somewhat experimental project!

Best Regards

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C40B Combinatorial chemistry

Classification subgroups

1/00	synthesis characterised by chemical nature of the compound library produced
3/00	apparatus specially adapted for use in the synthesis of chemical libraries
5/00	screening, methods specially adapted for use in screening of chemical libraries
7/00	identification of active compounds present in chemical libraries
9/00	combinatorial chemistry subjects not covered by 1/00 to 7/00

C40B Combinatorial chemistry

Subclass definitions

This subclass is primarily concerned with combinatorial chemistry, *ie* the creation of large populations of compounds *en masse* (known as a chemical or combinatorial library). Combinatorial synthesis may be followed by screening for desired activity and identification of individual compounds in the chemical library.

In this subclass the following terms are used with the following meanings:

Combinatorial chemistry: the systematic and repetitive connection of a set of different `building blocks` of varying structures to each other to yield a large array of diverse molecular entities

Screening: the process of determining whether compounds in a chemical library have a desired chemical or biological activity, *without* necessarily identifying the precise chemical nature of the compound(s) being screened

Iterative deconvolution: a method of identifying compounds in a chemical library involving the successive comparison (eg for activity) of an unknown compound with each of a set of sub-libraries, each sub-library having a fixed, known sub-unit in one of the positions, the set covering all possible sub-units for each other position.
Example:
Consider a library of 100 different esters of formula R_1-CO_2-R_2, formed by the reaction of 10 different carboxylic acids of formula R_1-CO_2H with 10 different alcohols of formula R_2-OH, and where one ester of highest activity is detected.

Iterative deconvolution, is used to find the highest activity ester, as follows:

10 sub-libraries of formula R_1-CO_2-R_2 are formed, each being formed from **one** of the 10 acids R_1-CO_2H, and all 10 of the alcohols R_2-OH, thus each sub-library has 10 members and R_1 is known ($R_1$is the fixed, known sub-unit). The most active sub-library tells us which R_1 is likely to be present in the most active ester in the 100 member library.

Then 10 further sub-libraries are formed, each being formed from **one** of the 10 alcohols R_2-OH, and all 10 of the acids R_1-CO_2H thus each sub-library has 10 members and R_2 is known. The most active sub-library tells which R_2 is likely to be present in the most active ester in the 100 member library.

Thus the identity of the highest activity ester is suggested by the result of the iterative deconvolution. (It should be noted that the most active ester need not be the ester corresponding to the R_1 and R_2 sub-libraries showing highest activity - iterative deconvolution is not necessarily definitive.)

C40B Combinatorial chemistry

Classification definitions for main group 1/00 - synthesis characterised by chemical nature of the compound library produced

Chemical natures including:-

inorganic libraries

peptide libraries (*including* polypeptide and protein libraries)

amide-linked oligomeric libraries

nucleic acid libraries

oligomeric or polymeric libraries

synthesis characterised by chemical nature of the compound library produced non-oligomeric organic libraries

C40B Combinatorial chemistry

Classification definitions for subgroup 5/00 - screening, methods specially adapted for use in screening of chemical libraries

Screening is defined as the process of determining whether compounds in a chemical library have a desired chemical or biological activity, *without* necessarily identifying the precise chemical nature of the compound(s) being screened

C40B Combinatorial chemistry

Classification definitions for subgroup 7/00 - identification of active compounds present in chemical libraries

7/00 includes identification through means dependent on the particular synthetic methodology used, e.g. :-

identification by position in space, *eg* by use of grids of phials

identification by tagging, ie association with an identifiable moiety (*eg* using nucleotides or radioactive markers)

identification by iterative deconvolution

7/00 also includes identification through means through means not dependent on particular synthetic methodology, e.g.:-

spectroscopy

[End of Annex and of document/
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