

C40B

COMBINATORIAL CHEMISTRY; LIBRARIES, e.g. CHEMICAL LIBRARIES, IN SILICO LIBRARIES

Definition statement

This place covers:

Methods of making libraries, e.g. combinatorial synthesis;

In silico or virtual conception of libraries; in silico or virtual libraries;

Chemical or biological libraries and modifications thereof, i.e. chemically, biologically or physically modified, e.g. proteins, DNAs, antibodies, specific chemicals;

Methods of screening libraries or subsets thereof for a desired activity or property, e.g. binding ability;

Methods specially adapted for identifying the exact nature, e.g. chemical structure of a particular library member;

Apparatus specially adapted for use in combinatorial chemistry or library technology to identify library members, to screen libraries or to synthesize libraries; integrated apparatus specially adapted for performing any combination of these three tasks;

Tags or linkers specially adapted for use in combinatorial chemistry or library technology;

Other process or products specially adapted for combinatorial chemistry or libraries.

Relationships with other classification places

Individual library members must be classified in the appropriate places elsewhere in CPC, e.g. in Section [C](#), according to established procedure, e.g. last place rule priority. Subject matter that has a wider utility and may also be used outside combinatorial chemistry, e.g. solid supports and linkers of general utility in solid phase synthesis, general reagents, is classified in the appropriate places elsewhere in CPC, e.g. Section [C](#).

Methods or apparatus covered by this subclass are also classified for their biological, chemical, physical or other features in the appropriate places in ECLA, if such features are of interest, e.g.

Biocides [A01N](#)

Preparations for medical, dental or toilet purposes [A61K](#)

Therapeutic activity of compounds [A61P](#)

Separation [B01D](#)

Chemical or physical processes, e.g. catalysis; Apparatus therefor [B01J](#)

Chemical or physical laboratory apparatus [B01L](#)

Shaped plastics [B29](#)

Inorganic, organic or organic macromolecular compounds; Methods of preparation or separation thereof [C01](#), [C07](#), [C08](#)

Biochemistry, microbiology, enzymology including microorganisms or enzymes, preparing them, using them to synthesize compounds or compositions; Measuring or testing processes involving microorganisms or enzymes; Mutation or genetic engineering [C12](#)

Metal alloys [C22](#)

Chemical or physical analysis [G01N](#)

Physical measurements methods; Apparatus therefore [G01R](#), [G01T](#)

Photomechanical methods [G03F](#)

Electrical digital data processing [G06F](#)

Data processing [G06K](#)

Image data processing [G06T](#)

Displaying; Advertising [G09F](#)

Special rules of classification

In this subclass, at each level of indentation, in the absence of an indication to the contrary, classification is made in the first appropriate place.

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere (see "Relationship between large subject matter areas" of this subclass and "References relevant to classification in this subclass" of the main groups)

[C12N 15/1034](#) - [C12N 15/1093](#) always take precedence over [C40B](#).

[C40B](#) is rarely used for search and classification as [C40B](#) is inconsistent in most areas to which it relates i.e. [G01N](#), [C12N](#), [B01J](#) and [C07](#). If [C40B](#) is used at all, it is used primarily as an indexing code to identify that there is some combinatorial chemistry aspect present in a document and there will always be further symbols from [G01N](#), [C12N](#), [B01J](#) and [C07](#) present.

Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

Array	Set of compounds maintained in a specified spatial distribution e.g. in the wells of a 96-well plate, in pins held in a rack or at the tip of optical fibers arranged in a bunch.
Biochemical method	Process involving the use of microorganisms, enzymes, vectors or antibodies, any biomolecular processes in vivo or in vitro.
Chemical Evolution Process	Process using in vitro selection systems that evolve to enrich mixtures of chemical compounds in those components having selected properties. The terminology "directed molecular evolution" is commonly employed when the process is applied to mixtures of macromolecules (e.g. RNA aptamers). Selected compounds are then amplified ("copied") using biochemical methods (e.g. enzymatic reverse transcription of RNA aptamers to DNA, PCR amplification and finally retranscription to RNA); This concept has been adapted to organic chemistry and opened a new branch of combinatorial chemistry named "dynamic combinatorial chemistry" wherein the enrichment in the (usually low-molecular weight) compounds having a selected property results from the equilibration process that carries out a preferential destruction and recycling of unselected compounds.

Coding/encoding	Strategy whereby a surrogate analyte is associated with each member of a library in order to record its structure and/or the reaction sequence used for its preparation. This is usually achieved by the use of tags/labels attached to the particles of solid support on which the library members are assembled.
Combinatorial library	A set of organic or inorganic compounds, plasmids, microorganisms, vectors or biopolymers, e.g. polynucleotides, proteins (a library) prepared by combinatorial synthesis. May consist of a collection of pools or sub-libraries. The sets can be in the form of arrays or mixtures.
Combinatorial synthesis	Combinatorial synthesis is the preparation of sets of diverse entities by the combination of sets of chemical building blocks and monomers, e.g. reagents.
Contained in	A library contained in a microorganism, a cell or a vector is a library the members of which are present in the respective biochemical, e.g. in a plasmid.
Decoding	Method enabling the determination of the structure of a library member and/or the reaction sequence leading to its preparation, consisting in "reading" (e.g. determining the structure of) a surrogate analyte (code, tag, label) associated with said library-member.
Deconvolution	Process consisting of fractionating (normally by resynthesis, or by elaborating a partial library) a pool with some level of the desired activity to give a set of smaller pools. See also iterative deconvolution.
Directed Molecular Evolution	Directed Molecular Evolution is a process for enriching a library in members having a property or activity of interest. It involves cycles of taking a library, subjecting it to a screen to select for the desired property or activity, amplifying the "hits" to provide the starting library for the subsequent cycle. "Mutations" may be introduced at the amplification stage in order to increase the diversity of the library. This subject matter involves aspects of creating and screening libraries.
Displayed by	A library displayed by a microorganism is a library present at the surface of such a microorganism, e.g. of a bacteria. See for example Nature Biotechnology (1997), 15, pages 29-34: "Display of heterologous proteins on the surface of microorganisms: from the screening of combinatorial libraries to live recombinant vaccines".
Dynamic Library	Collection of compounds (in solution) in dynamic equilibrium (i.e. constantly changing). If the composition of the library is altered by the presence of a target which selectively binds certain library members, then shifting of the equilibrium will lead to an increase in the amount of those components which bind to the target with relatively high affinity. A dynamic library contains all the potentially possible combinations of the components undergoing dynamic random connection, whether these combinations are or are not actually present in the conditions used. It is a virtual library. A real entity is generated in the presence of the target.

Fluorous Synthesis	Approach for solution phase synthesis which takes advantage of the ability of highly fluorinated groups to partition out of aqueous and most organic solutions into a third phase consisting in a fluorinated solvent. The fluorinated side chain can act as a soluble support for synthesis.
Identifying	Determining the exact nature, e.g. chemical structure or sequence listing, of a particular library member or of a particular subset of library members.
In silico library	A library which has no physical existence, being constructed solely in electronic form or on paper. It is one type of virtual library. The building blocks required for such a library may not exist, and the chemical steps for creating such a library may not have been tested. These libraries are used in the design and evaluation of possible libraries.
"Integrated" apparatus	Apparatus specifically designed for performing at least two different operations, e.g. synthesis and screening.
Iterative deconvolution	Method for the identification of active library members consisting in repeating the deconvolution strategy a certain number of times. Usually the initial library is divided into non-overlapping subsets. The subsets are tested (screened) separately, and the one with the greatest activity is identified. This subset is re-synthesized as a collection of simpler subsets which are tested for activity. The process is repeated until a unique library-member with (ideally) a high level of activity is identified.
Library	A library is a created collection of a plurality of compounds, microorganisms or other substances, all being of the same type . The collection is useful as a test vehicle for determining which of its members or its subsets of members possess activities or properties of interest. A library might for example exist as: -a solution -a physical admixture -an ordered or unordered array-a plurality of members present on a support and affixed thereto, e.g. by chemical bonding, by physical attractive forces or by coating.
Liquid-phase synthesis	In the context of C40B , this wording covers both solution phase syntheses (i.e. reactions involving only one liquid phase) as well as syntheses in multiple liquid phase systems (i.e. involving more than one liquid phase). The latter concern for instance syntheses performed on a liquid macromolecular compound such as PEG (polyethylene glycol), on dendrimers, or wherein a fluorocarbon phase is present in the system (fluorous synthesis).
Microorganisms	Bacteria, actinomycetales, fungi (e.g. yeast), virus, human, animal, or plant cells, tissues, protozoa or unicellular algae.
Particular attachment method	Specific method of attachment focusing on the way molecules are bound to the solid or liquid support, e.g. by means of electrostatic interactions, formation of covalent bonds by cycloaddition reactions or by irradiation.
Resin capture	Method consisting in contacting the reaction medium with a solid support after a reaction performed in solution, in order to attach the reaction product to the resin and thus collect it easily.
Safety-Catch Linker	A linker which is cleaved by performing two different reactions instead of only one, thus providing greater control over the timing of compound release. In practice, the resin is "activated" before the actual cleavage takes place (e.g. cleavage by nucleophilic displacement of a previously alkylated sulfonamide resin).

Screening	Determining whether a library contains a member or members which have a particular property or activity of interest.
Solid-phase synthesis	Synthetic process wherein the reactions are performed on a solid support, usually in the presence of a solvent, i.e. wherein one or more library building blocks are bound to a solid support (e.g. polymer, resin, glass beads) during library creation.
Solid support	Insoluble, functionalized or not, material, e.g. polymers, glass to which library members or other reagents may be attached (often via a linker) allowing library members to be readily separated (by filtration, centrifugation, etc.) from excess reagents, soluble reaction by-products or solvents.
Solution-phase synthesis	Synthesis performed in solution, i.e. wherein the reactants and reagents are all soluble in the reaction medium (irrespective of the fact that, for instance, a supported catalyst is used during the reaction). It is also called "synthesis in solution".
Traceless Linker	Linker which does not leave any residue on the cleaved compound, i.e. which is replaced by a hydrogen atom.
Virtual library	A library which has no physical existence. This terminology encompasses two different types of libraries: in silico libraries and dynamic libraries.

C40B 10/00

Directed molecular evolution of macromolecules, e.g. RNA, DNA or proteins

Special rules of classification

Classification in [C12N 15/1058](#) takes precedence over classification in [C40B 10/00](#)

C40B 20/00

Methods specially adapted for identifying library members

Definition statement

This place covers:

Methods specially adapted for identifying library members.

Relationships with other classification places

The methods classified here must also be classified in the appropriate places elsewhere in CPC for relevant aspects:

Chemical or physical laboratory apparatus: [B01L](#)

Chemical or physical analysis: [G01N](#)

Physical measurements methods; Apparatus therefore [G01R](#), [G01T](#)

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

General synthesis of combinatorial arrays	B01J 19/0046
-------------------------------------------	------------------------------

Means for coding or tagging apparatus or reagents	B01J 2219/0054 and lower subgroups
Spatial configuration of library members on arrays	B01J 2219/00603 and lower subgroups
Isolating an individual clone by screening libraries	C12N 15/1034

Special rules of classification

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere (see "Relationship between large subject matter areas" of this subclass and "References relevant to classification in this subclass" of the main groups)

[C12N 15/1034](#) always takes precedence over [C40B 20/00](#)

C40B 30/00

Methods of screening libraries

Definition statement

This place covers:

Methods for determining whether a library contains a member or members which have a particular property or activity of interest.

Relationships with other classification places

The methods classified here must also be classified in the appropriate places elsewhere in the IPC for relevant aspects:

Chemical or physical laboratory apparatus: [B01L](#)

Chemical or physical analysis: [G01N](#)

Measuring or testing processes involving enzymes, nucleic acids or microorganisms : [C12Q](#)

Physical measurements methods; Apparatus therefore [G01R](#), [G01T](#)

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

General synthesis of combinatorial arrays	B01J 19/0046
Means for coding or tagging apparatus or reagents	B01J 2219/0054
Spatial configuration of library members on arrays	B01J 2219/00603
Screening of catalysts is often also classified in	B01J 2219/00747
Isolating and individual clone by screening libraries	C12N 15/1034
Screening libraries presented on the surface of microorganism	C12N 15/1037
Proteomic analysis of sub-sets of protein mixtures	G01N 33/6842
Methods of protein analysis involving mass spectrometry	G01N 33/6848

Chemical aspects of mass spectrometric analysis of biological material

G01N 2560/00

Special rules of classification

When classifying in this group, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere

This is particularly applicable to sub-group [C40B 30/04](#) where classification is almost always possible and essential in one or more places in the range [G01N 33/53-G01N 33/98](#).

Similarly for sub-group [C40B 30/06](#) classification is also required in one or more places in the range [G01N 33/5008-G01N 33/5088](#) or [C12Q 1/025](#).

[C12N 15/1034](#) always take precedence over [C40B 30/00](#)

C40B 30/06

by measuring effects on living organisms, tissues or cells

Definition statement

This place covers:

Screening libraries for compounds with a biological activity, e.g. for drug discovery purposes. The screening is achieved by measuring the effect of the library members on living organisms or parts thereof. A typical example is the testing effect of library members on tumour cell growth for anti-cancer drug development.

C40B 30/08

by measuring catalytic activity

Definition statement

This place covers:

Screening libraries for compounds including enzymes with catalytic activity

C40B 40/00

Libraries per se, e.g. arrays, mixtures

Definition statement

This place covers:

Sets of organic or inorganic compounds, plasmids, microorganisms, vectors, biopolymers or biomolecules, prepared by combinatorial synthesis.

The sets can be in the form of arrays or mixtures.

Relationships with other classification places

The libraries classified here must also be classified in the appropriate places elsewhere in CPC:

Plasmids, microorganisms or vectors: Classifying in [C12N 15/1037](#) takes precedence over the classification in [C40B 40/02](#)

Organic compounds not covered by the sub-groups [C40B 40/06](#) - [C40B 40/16C07C](#) or [C07D](#)

Nucleotides, polynucleotides, RNA or DNA: [C12N 15/1034](#) - [C12N 15/1093](#) always take precedence over [C40B 40/06](#) and [C40B 40/08](#).

DNA chip: [B01J 19/0046](#); [C12Q 1/6837](#)

Peptides or polypeptides: [C07K 1/047](#) (peptide libraries)

Saccharides: [C07H](#)

Polysaccharides: [C08B](#)

Macromolecular compounds not covered by the groups [C40B 40/06](#) - [C40B 40/12:C08F](#) (polymers)

Metal-containing organic compounds: [C07F](#), [B01J](#) (catalysts)

Inorganic compounds or materials: [C07F](#), [B01J](#) (catalysts)

Compounds attached to a solid support must also be given the Indexing Code [C07B 2200/11](#)

References

Limiting references

This place does not cover:

Supported catalysts used in combinatorial synthesis if the catalyst itself is not considered a combinatorial library	B01J 23/00 - B01J 35/12
Isolating an individual clone by screening libraries	C12N 15/1034 - C12N 15/1093
Screening libraries presented on the surface of microorganisms	C12N 15/1037

Informative references

Attention is drawn to the following places, which may be of interest for search:

Simultaneous synthesis of different peptide species; Peptide libraries:	C07K 1/047
-------------------------------------------------------------------------	----------------------------

Special rules of classification

[C12N 15/1034](#) - [C12N 15/1093](#) always take precedence over [C40B 40/06](#) and [C40B 40/08](#).

[C12N 15/1034](#) - [C12N 15/1093](#) always take precedence over [C40B 40/02](#), [C40B 40/06](#) and [C40B 40/08](#)

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere

Classification is made in the first appropriate place, e.g. libraries containing organic and inorganic compounds are classified in [C40B 40/04](#)

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

C40B 50/00

Methods of creating libraries, e.g. combinatorial synthesis

Definition statement

This place covers:

Methods specially adapted for creating libraries, e.g. split-pool synthesis, solid phase synthesis, creating gradient libraries.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

General methods for combinatorial chemistry or making combinatorial arrays	B01J 19/0046
----------------------------------------------------------------------------	------------------------------

Special rules of classification

Classification in [C12N 15/1093](#) takes precedence over classification in [C40B 50/00](#)

C40B 50/04

using dynamic combinatorial chemistry techniques

Definition statement

This place covers:

Methods specially adapted for creating library members using dynamic combinatorial chemistry techniques (DCC). Dynamic combinatorial chemistry is a reversible assembly process, its constituents being molecular or supramolecular. The library is produced from a set of reversibly-interchangeable components (collection of compounds).

Special rules of classification

See corresponding header in [C40B 50/00](#)

C40B 50/06

Biochemical methods, e.g. using enzymes or whole viable microorganisms

Definition statement

This place covers:

Methods specially adapted for synthesizing library members using biochemical methods, e.g. using enzymes or whole viable microorganisms

Special rules of classification

See corresponding header in [C40B 50/00](#)

C40B 50/08

Liquid phase synthesis, i.e. wherein all library building blocks are in liquid phase or in solution during library creation; Particular methods of cleavage from the liquid support

Definition statement

This place covers:

Liquid phase synthesis, i.e. wherein all library building blocks are in liquid phase or in solution during library creation; Particular methods of cleavage from the liquid support i.e. once the libraries are created, methods of cleaving the compounds from the liquid support.

Special rules of classification

See corresponding header in [C40B 50/00](#)

C40B 50/14

Solid phase synthesis, i.e. wherein one or more library building blocks are bound to a solid support during library creation; Particular methods of cleavage from the solid support

Definition statement

This place covers:

Solid phase synthesis, i.e. wherein one or more library building blocks are bound to a solid support during library creation; Particular methods of cleavage from the solid support i.e. once the libraries are created, methods of cleaving the compounds from the solid support.

Special rules of classification

See corresponding header in [C40B 50/00](#)

C40B 60/00

Apparatus specially adapted for use in combinatorial chemistry or with libraries

Definition statement

This place covers:

Apparatus specially adapted for use in combinatorial chemistry or with libraries.

Such apparatus may deal with synthesis, screening, identification of library members, or a combination of these functions.

Relationships with other classification places

The apparatuses classified here must also be classified in the appropriate places elsewhere in CPC:

Apparatus for chemical or physical processes: [B01J](#)

Chemical or physical laboratory apparatus: [B01L](#)

Apparatus for screening, sampling or analysis: [G01N](#)

Physical measurements methods; Apparatus therefore: [G01R](#), [G01T](#)

References

Application-oriented references

Examples of places where the subject matter of this place is covered when specially adapted, used for a particular purpose, or incorporated in a larger system:

Apparatus for combinatorial synthesis	B01J 19/0046
Special features of apparatus for combinatorial synthesis	B01J 2219/00274 and lower groups

Special rules of classification

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere

The first-place rule is applied

Apparatus classified in [C40B 60/02](#), [C40B 60/06](#), [C40B 60/08](#) or [C40B 60/14](#) should receive classification for additional information in [B01J 2219/00274](#) and lower subgroups.

C40B 70/00

Tags or labels specially adapted for combinatorial chemistry or libraries, e.g. fluorescent tags or bar codes

Definition statement

This place covers:

Tags or labels specially adapted for combinatorial chemistry or libraries, e.g. fluorescent tags or bar codes.

Relationships with other classification places

The tags/labels classified here must also be classified in the appropriate places elsewhere in CPC:

Tags/labels should be also classified in the appropriate class in CPC, according to established procedure, e.g. organic compounds are also classified in the appropriate place in section [C](#).

Production of labelled immunochemical (including materials having complementary binding properties) test materials, [G01N 33/532](#) or subgroups.

Use of labelled substances in immunoassays (including complementary binding assays), [G01N 33/58](#) or subgroups.

Tags or labels attached to a solid support must also be given the symbol [C07B 2200/11](#) .

References

Limiting references

This place does not cover:

Tags or labels which are not specially adapted/used in combinatorial chemistry	appropriate class elsewhere in CPC, e.g. section C
--------------------------------------------------------------------------------	--------------------------------------------------------------------

Informative references

Attention is drawn to the following places, which may be of interest for search:

Analysing compounds using physical methods, e.g. spectroscopy	G01N 33/00
---------------------------------------------------------------	----------------------------

Special rules of classification

The last-place rule applies.

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere

[C12N 15/1065](#) takes precedence over classification in [C40B 70/00](#)

Synonyms and Keywords

In patent documents, the following abbreviations are often used:

RF tag	radio frequency tag
--------	---------------------

C40B 80/00**Linkers or spacers specially adapted for combinatorial chemistry or libraries, e.g. traceless linkers or safety-catch linkers****Definition statement**

This place covers:

Linkers or spacers specially adapted for combinatorial chemistry or libraries, e.g. traceless linkers, photolabile linkers, safety-catch linkers or cleavable linkers.

Linkers or spacers attached to a solid support are also classified here.

Linkers or spacers attached to a solid support must also be given the symbol [C07B 2200/11](#).

Relationships with other classification places

Linker or spacer molecules classified here must also be classified in the appropriate places elsewhere in CPC, e.g. in section [C](#). linkers and spacers attached to a solid support are classified according to the classification of the linker or spacer, the solid support is disregarded for the purpose of classification.

References**Application-oriented references**

Examples of places where the subject matter of this place is covered when specially adapted, used for a particular purpose, or incorporated in a larger system:

The manner of attachment to the support and the nature of the support	B01J 2219/00605
Linking groups for attachment of ligands to carriers for use in immunoassays (including complementary binding assays)	G01N 33/54353

Special rules of classification

The last-place rule applies.

When classifying in this subclass, additional classifications are made for subject matter which is considered invention information or is considered of interest for search purposes.

Please note that it is of vital importance to the completeness of other places of classification that documents are not only classified in [C40B](#), but wherever possible also elsewhere

For the main group [C40B 80/00](#) classification is often also required in the subgroup [G01N 33/54353](#)

Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

Linker: a bi-, or multifunctional molecule, which can be bound to the carrier linker	or multifunctional molecule, which can be bound to the carrier phase and offers a binding site for the coupling of desired molecules so that chemical reactions can be carried out.
Spacer	Molecule which is located between the carrier and the linker.
See also glossary at subclass level	C40B

C40B 99/00

Subject matter not provided for in other groups of this subclass

Definition statement

This place covers:

Subject matter not provided for in other groups of this subclass

References

Limiting references

This place does not cover:

All other (sub-)groups in C40B	C40B 10/00 - C40B 80/00
------------------------------------------------	---------------------------------------------------------

Special rules of classification

This group is preferably not used.

Since this group is normally not used in search, other classes must be assigned to documents classified in this group.