

CLASS 506, COMBINATORIAL, CHEMISTRY TECHNOLOGY: METHOD, LIBRARY, APPARATUS

SECTION I - CLASS DEFINITION

GENERAL STATEMENT OF THE CLASS SUBJECT MATTER

This is the specific class for combinatorial chemistry technology, which includes the following subject matter:

A. Methods specially adapted for identifying the exact nature (e.g., chemical structure, etc.) of a particular library member.

B. Methods of screening libraries or subsets thereof for a desired activity or property (e.g., binding ability, etc.).

C. Chemical or biological libraries and modifications thereof (i.e., chemically, biologically, or physically modified).

D. In silico or virtual libraries and their conception.

E. Methods of making libraries (e.g., combinatorial synthesis, etc.).

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

G. Tags, labels, linkers, or spacers specially adapted for use in combinatorial chemistry or library technology.

H. Other processes or products specially adapted for combinatorial chemistry or libraries.

SECTION II - SUBCLASS REFERENCES TO THE CURRENT CLASS

SEE OR SEARCH THIS CLASS, SUBCLASS:

- 1, for a combinatorial chemistry process involving the process of directed molecular evolution of macromolecules such as RNA, DNA, and proteins.
- 2, through 6, for methods that are specially adapted for identifying the nature of a specific library member.

- 7, through 12, for methods of screening a library for members that have a particular property or activity of interest.
- 13, through 22, for libraries, per se, based on their chemical or biological nature.
- 23, through 32, for methods of creating or synthesizing libraries including in silico, biochemical, and chemical methods.
- 33, through 40, for apparatus specially adapted for use in identifying, screening, or creating libraries.
- 41, for a tag or label that is specially adapted for used in a combinatorial chemistry process.
- 42, for a linker or spacer that is specially adapted for use in a combinatorial chemistry process.
- 43, for combinatorial chemistry technology not provided for elsewhere.

SECTION III - REFERENCES TO OTHER CLASSES

SEE OR SEARCH CLASS:

- 73, Measuring and Testing, for processes and apparatus for determining a physical property of what is being tested.
- 204, Chemistry: Electrical and Wave Energy, for a process of preparing compounds or elements involving chemical reactions brought about by electric or wave energy or an electrostatic field or electrical discharge and apparatus therefore.
- 260, Chemistry of Carbon Compounds, subclass 665 for organic compounds containing a metal other than a heavy metal or aluminum bonded to carbon.
- 420, Alloys or Metallic Compositions, for alloys containing metal or metallic compositions which contain a continuous phase of metal and methods of making same not provided for elsewhere and elemental metal, per se.
- 422, Chemical Apparatus and Process Disinfecting, Deodorizing, Preserving, or Sterilizing, subclasses 50 through 570 for apparatus for performing an analysis which involves a chemical or physical reaction not elsewhere provided for and subclasses 129-242 for carrying out chemical reactions.
- 423, Chemistry of Inorganic Compounds, for inorganic compounds and nonmetallic elements and processes of producing by a chemical reaction.
- 424, and 514, Drug, Bio-Affecting and Body Treating Compositions, for compositions used for testing of living organisms; preventing, allevi-

- ating, treating, or curing abnormal and pathological conditions of the living body; and maintaining, increasing, decreasing, limiting, or destroying a physiologic body function, etc.
- 435, Chemistry: Molecular Biology and Microbiology, for micro-organisms, vectors, and enzymes, per se; methods of producing them; testing processes involving micro-organisms and enzymes; and apparatus therefor not specially adapted for combinatorial chemistry technology.
- 436, Chemistry: Analytical and Immunological Testing, subclasses 500 through 542 for immunological tests and related subject matter, and for processes of analysis of chemical properties of a sample, physiological effect of a sample, or chemical determination of a physical property of a sample not specially adapted for combinatorial chemistry technology.
- 502, Catalyst, Solid Sorbent, or Support Therefor: Product or Process of Making, subclasses 100 through 355 for a catalyst or precursor therefor and subclasses 400-438 for a solid sorbent.
- 504, Plant Protecting and Regulating Compositions, for compositions for treating living terrestrial and aquatic plants or their habitats for the purpose of stimulating or inhibiting growth or any regulating action on plant growth through chemical modification of plant metabolism.
- 520, Synthetic Resins or Natural Rubbers, subclass 1 for the residual home for compositions containing a solid synthetic resin or natural rubber, preparation, or treatment thereof.
- 521, Synthetic Resins or Natural Rubbers, for ion-exchange polymers, processes of reclaiming a solid synthetic resin, and for cellular synthetic resins.
- 522, Synthetic Resins or Natural Rubbers, for processes of preparing or treating a solid polymer utilizing wave energy, for compositions to be polymerized by wave energy wherein said composition contains a rate-affecting material, or for compositions to be modified by wave energy wherein said composition contains a rate-affecting material.
- 523, and 524, Synthetic Resins or Natural Rubbers, for solid synthetic resins or specified intermediate condensation products admixed with a nonreactant material.
- 525, Synthetic Resins or Natural Rubbers, for certain combinations of polyesters and certain reactable materials, for blends of solid synthetic resins, and for chemically modified solid synthetic resins.
- 526, Synthetic Resins or Natural Rubbers, for certain manipulative processes which are generic to both ethylenic polymers and to condensation polymers, and also provides for polymers derived from ethylenic monomers only.
- 527, Synthetic Resins or Natural Rubbers, for solid synthetic resins derived from at least one saturated material and certain special reactants (e.g., carbohydrates, proteins, natural resins, lignin, tannin, bituminous material, etc.).
- 528, Synthetic Resins or Natural Rubbers, for solid synthetic resins derived from plant material of unknown constitution or from at least one non-ethylenic reactant, and also for processes of treating a polymer either derived from ethylenic or nonethylenic reactants wherein chemical bonds in the polymer are left unaffected.
- 530, Chemistry: Natural Resins or Derivatives; Peptides or Proteins; Lignins or Reaction Products Thereof, subclasses 200 through 233 for natural resins or derivatives, subclasses 300-427 for peptides or proteins, and subclasses 500-507 for lignins or derivatives.
- 534, Organic Compounds, for noble gases, radioactive or rare earth metal compounds, and azo and diazo compounds.
- 536, Organic Compounds, for carbohydrates.
- 540, Organic Compounds, for heterocyclic carbon compounds.
- 544, Organic Compounds, for six-membered nitrogen hetero rings with two or more hetero atoms.
- 546, Organic Compounds, for six-membered hetero rings with one ring nitrogen.
- 548, Organic Compounds, for three-, four-, or five-membered nitrogen hetero rings.
- 549, Organic Compounds, for oxygen or sulfur hetero rings.
- 552, Organic Compounds, for azides, triphenylmethanes, quinones, hydroquinones, or steroids.
- 554, Organic Compounds, for fats or fatty derivatives.
- 556, Organic Compounds, for heavy metal, aluminum, or silicon compounds.
- 558, and 560, Organic Compounds, for different esters.
- 562, Organic Compounds, for acids, acid halides, acid anhydrides, or selenium and tellurium compounds.
- 564, Organic Compounds, for amino nitrogen compounds.
- 568, Organic Compounds, for boron, phosphorus, sulfur, or oxygen compounds.

- 570, Organic Compounds, for halogen compounds.
 585, Organic Compounds, for hydrocarbons and certain compositions containing hydrocarbons.
 702, Data Processing: Measuring, Calibrating, or Testing, subclasses 19 through 32 for apparatus and corresponding methods wherein the data processing system or calculating computer is designed for or utilized in a biological, biochemical, or chemical environment relating to a specific or generic measurement system, a calibration or correction system, or a testing system.
 703, Data Processing: Structural Design, Modeling, Simulation, and Emulation, subclass 11 and 12 for simulating a nonelectrical biological, biochemical, or chemical device or system.
 977, Nanotechnology, for cross-reference art collections relating to nanostructure; chemical compositions of nanostructure; devices that include at least one nanostructure; mathematical algorithms specifically adapted for modeling configurations or properties of nanostructure; methods or apparatus for making, detecting, analyzing, or treating nanostructure; and specified particular uses of nanostructure.

SECTION IV - GLOSSARY

Terms used throughout the schedule and definitions are to have the meaning ascribed below. Generally accepted or commonly used "art" terms retain their meaning found in their everyday usage and are not found in this glossary. Certain specialized terms are employed in these subclasses and these terms have been given definitions altered to meet the needs of this class. Some or all of the terms may be broader or more restricted, as well as different in meaning compared to normal usage.

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, etc.).

BIOCHEMICAL METHOD

Process involving the use of micro-organisms, enzymes, vectors, or antibodies.

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, etc.). 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, etc.). 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 OR ECODING

Strategy whereby a surrogate analyte is associated with each member of a library in order to record its structure or the reaction sequence used for its preparation. This is usually achieved by the use of tags or labels attached to particles or solid supports on which the library members are assembled.

COMBINATORIAL LIBRARY

A set of compounds (a library) prepared by combinatorial synthesis. This set may consist of a collection of pools or sublibraries.

COMBINATORIAL SYNTHESIS

Combinatorial synthesis is the preparation of sets of diverse entities by the combination of sets of chemical building blocks (e.g., reagents, etc.).

CONTAINED IN

A library "contained in" a micro-organism, a cell, or a vector is a library in which the members are present in the respective biological entity (e.g., in a plasmid, etc.).

DECODING

Method enabling the determination of the structure of a library member or the reaction sequence leading to its preparation, which method involves "reading" (e.g., determining the structure of, etc.) a surrogate analyte (e.g., code, tag, label, etc.) associated with said library member.

DECONVOLUTION

Process 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. Directed molecular evolution involves cycles of taking a library, subjecting it to a screen to select for the desired property or activity, and 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 micro-organism is a library present at the surface of such a micro-organism (e.g., of a bacteria, etc.).

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 comprising 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, etc.) 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. An in silico library 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, etc.).

ITERATIVE DECONVOLUTION

Method for the identification of active library members which involves repeating the deconvolution strategy a certain number of times. Usually the initial library is divided into nonoverlapping subsets. The subsets are tested or 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 a high level of activity is identified.

LIBRARY

A library is a created collection of a plurality of compounds, micro-organisms, or other substances. 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) a solution, (b) a physical admixture, (c) an ordered or unordered array, or (d) a plurality of members present on a support and affixed thereto (e.g., by chemical bonding, physical attractive forces, coating, etc.).

LIQUID-PHASE SYNTHESIS

This terminology 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 is concerned with syntheses performed on a liquid macromolecular compound such as polyethylene glycol (PEG), on dendrimers, or wherein a fluorocarbon phase is present in the system (fluorous synthesis).

MICRO-ORGANISMS

Bacteria; actinomycetales; single-celled fungi (e.g., yeast, etc.); 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, etc.).

RESIN CAPTURE

Method involving contacting the reaction medium with a solid support after a reaction is performed in solution in order to attach the reaction product to the resin and thus collect the reaction product 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, etc.).

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, etc.) during library creation.

SOLID SUPPORT

Insoluble, functionalized, polymeric material 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). Solution-phase synthesis is also known as "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.

SUBCLASSES**1 DIRECTED MOLECULAR EVOLUTION OF MACROMOLECULES (E.G., RNA, DNA, PROTEINS, ETC.):**

This subclass is indented under the class definition. Method wherein a library of macromolecules, such as nucleic acids or proteins, is enriched in members having a property or activity of interest and involves cycles of taking a library, subjecting it to a screen to select for the desired property or activity, and amplifying the "hits" to provide the starting library for the subsequent cycle.

- (1) Note. "Mutations" may be introduced at the amplification stage in order to increase the diversity of the library.
- (2) Note. Directed molecular evolution involves aspects of creating and screening libraries.
- (3) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 10/00.

2 METHOD SPECIALLY ADAPTED FOR IDENTIFYING A LIBRARY MEMBER:

This subclass is indented under the class definition. Method wherein the method is specially adapted to determine the exact nature (e.g., chemical structure, sequence listing, etc.) of a

particular library member or of a particular subset of library members.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 20/00.

SEE OR SEARCH CLASS:

435, Chemistry: Molecular Biology and Microbiology, subclasses 4 through 40.52 for testing processes involving micro-organisms and enzymes not specially adapted for combinatorial chemistry technology.

436, Chemistry: Analytical and Immunological Testing, subclasses 500 through 542 for immunological tests and related subject matter, and for processes of analysis of chemical properties of a sample, physiological effect of a sample, or chemical determination of a physical property of a sample not specially adapted for combinatorial chemistry technology.

3 Identifying a library member by its fixed physical location on a support or substrate: Method under subclass 2 wherein the exact nature of a library member is determined from its physical location in an array or arrangement.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 20/02.

4 Identifying a library member by means of a tag, label, or other readable or detectable entity associated with the library member (e.g., decoding process, etc.):

Method under subclass 2 wherein the exact nature of a library member to which a surrogate analyte (tag, label, etc.) is associated is determined by using the surrogate analyte which is attached to a solid support on which the library members are assembled to define the reaction path to which the solid support was exposed and hence imply the structure of a member of a library or the reaction sequence for its preparation.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 20/04.

5 Using an iterative deconvolution technique: Method under subclass 2 wherein the exact nature of a library member is determined by a method of screening of compound pools, identifying the active pool(s), resynthesizing and rescreening sublibraries (smaller pools), wherein the number of compounds in the sublibraries gets smaller and smaller, until only a single compound is present in each pool, thereby leading to the identification of the active library member(s).

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 20/06.

6 Direct analysis of a library member, per se, by a physical method (e.g., spectroscopy, etc.):

Method under subclass 2 wherein the exact nature of a library member is directly determined by a physical (nonchemical) method.

- (1) Note. Physical methods include mass spectroscopy, nuclear magnetic resonance (NMR), etc.
- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 20/08.

7 METHOD OF SCREENING A LIBRARY: This subclass is indented under the class definition. Method for determining whether a member or members of a library have a desired chemical, physical, or biological property or activity, without necessarily identifying the precise nature of the member or members being screened.

- (1) Note. A method of screening a library is provided for in this subclass if the method involves screening the library as a whole, and if the method recites a library-specific limitation. The library should be an intentionally created library testing set. The simple repetitive screening of an ordered array of subject materials in individual containers simultaneously or sequentially, without recitation of a library-specific limitation, would not meet this test.

- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/00.
- SEE OR SEARCH CLASS:
- 435, Chemistry: Molecular Biology and Microbiology, subclasses 4 through 40.52 for testing processes involving micro-organisms and enzymes not specially adapted for combinatorial chemistry technology.
- 436, Chemistry: Analytical and Immunological Testing, subclasses 500 through 542 for immunological tests and related subject matter, and for processes of analysis of chemical properties of a sample, physiological effect of a sample, or chemical determination of a physical property of a sample not specially adapted for combinatorial chemistry technology.
- 8 In silico screening:**
Method under subclass 7 wherein the members of a library are selected by evaluating their desirability in a computational model.
- (1) Note. In silico screening is also known as virtual screening.
- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/02.
- 9 By measuring the ability to specifically bind a target molecule (e.g., antibody-antigen binding, receptor-ligand binding, etc.):**
Method under subclass 7 wherein the members of a library are selected for their ability to principally attach to a target entity such as in antibody-antigen binding, biospecific ligand binding, etc.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/04.
- 10 By measuring the effect on a living organism, tissue, or cell:**
Method under subclass 7 wherein members of a library are selected for their ability to produce a change in a living organism, tissue, or cell
- such as death, increased production of a product, etc.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/06.
- 11 By measuring catalytic activity:**
Method under subclass 7 wherein members of a library are selected for their ability to catalyze reactions.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/08.
- 12 By measuring a physical property (e.g., mass, etc.):**
Method under subclass 7 wherein members of a library are selected for a specific physical (nonchemical) property such as density, refractive index, mass, etc.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 30/10.
- 13 LIBRARY, PER SE (E.G., ARRAY, MIXTURE, IN SILICO, ETC.):**
This subclass is indented under the class definition. Subject matter which is a created collection of a plurality of chemical compounds, biological entities (e.g., plasmid, bacterium, yeast cell, animal cell, etc.), or other materials wherein the collection is treated as a unit.
- (1) Note. The collection is useful as a test vehicle for determining which of its members possess(es) a useful property or activity.
- (2) Note. A library may exist as (a) a solution, (b) a physical admixture, (c) an ordered or unordered array, (d) a plurality of members present on a support and affixed thereto by chemical bonding, by physical attractive forces, or by coating, or (e) virtual or in silico (i.e., a library which is constructed solely in electronic form or on paper and has no physical existence).
- (3) Note. A natural product (e.g., plant extracts, etc.) is not considered as being

a library, per se, for the purposes of this subclass, except where plural natural products are intentionally combined to make a library.

- (4) Note. Virtual or in silico libraries are classified as if they are physically existing entities (e.g., a virtual gene library is classified with the gene libraries, etc.).
- (5) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/00.

14 Library contained in or displayed by a micro-organism (e.g., bacteria, animal cell, etc.) or library contained in or displayed by a vector (e.g., plasmid, etc.) or library containing only micro-organisms or vectors:

Library under subclass 13 wherein the library members are enclosed in or found on the surface of a micro-organism or a vector such as a plasmid, or the library members are a grouping of micro-organisms or vectors (e.g., virus library, plasmid library, etc.).

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/02.

SEE OR SEARCH CLASS:

435, Chemistry: Molecular Biology and Microbiology, subclasses 235.1 through 239 for virus or bacteriophage, per se; subclasses 243-261 for micro-organism, per se; subclass 320.1 for virus vector or bacteriophage vector, per se; subclasses 325-408 for animal cell, per se; and subclasses 410-431 for plant cell, per se.

15 Library containing only organic compounds:

Library under subclass 13 wherein the library members are solely organic compounds.

- (1) Note. An organic compound is defined as satisfying one of the following criteria: (a) at least two carbon atoms bonded to each other, or (b) one carbon atom bonded to at least one hydrogen atom or halogen atom, or (c) one carbon atom bonded to at least one nitrogen atom by a single or double bond. Exceptions to the

above criteria are compounds consisting of only carbon atoms (e.g., fullerenes, etc.), cyanogen, cyanogen halides, cyanamide, metal carbides, hydrocyanic acid, isocyanic acid, isothiocyanic acid, fulminic acid, and salts of the previously mentioned acids. These exceptions are considered to be inorganic compounds for classification purposes.

- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/04.

16 Nucleotides or polynucleotides, or derivatives thereof:

Library under subclass 15 wherein the library members are nucleotides or polynucleotides (e.g., nucleic acids, oligonucleotides, etc.).

- (1) Note. A nucleotide is a phosphorylated nucleoside.
- (2) Note. Polynucleotides, also called nucleic acids, are covalently linked series of nucleotides in which the 3i position of the pentose of one nucleotide is joined by a phosphodiester group to the 5i position of the next.
- (3) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/06.

SEE OR SEARCH CLASS:

536, Organic Compounds, subclasses 22.1 through 29.13 for N-glycosides, per se, including nucleotides, nucleic acids, oligonucleotides, etc.

17 RNA or DNA which encodes proteins (e.g., gene library, etc.):

Library under subclass 16 wherein the library members are ribonucleic acids or deoxyribonucleic acids which carry the genetic code for making a specific protein.

- (1) Note. An example of an encoding nucleic acid library is a gene library.
- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/08.

18 Peptides or polypeptides, or derivatives thereof:

Library under subclass 15 wherein the library members are compounds containing two or more amino acids joined covalently by peptide bonds (e.g., dipeptides, proteins, etc.).

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/10.

SEE OR SEARCH CLASS:

530, Chemistry: Natural Resins or Derivatives; Peptides or Proteins; Lignins or Reaction Products Thereof, subclasses 300 through 427 for peptides or proteins, per se.

19 Saccharides or polysaccharides, or derivatives thereof:

Library under subclass 15 wherein the library members are carbohydrates.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/12.

SEE OR SEARCH CLASS:

536, Organic Compounds, for carbohydrates, per se.

20 Macromolecular compounds (e.g., synthetic resins, rubber, etc.):

Library under subclass 15 wherein the library members are polymer compounds which are made up of many smaller monomer units joined together chemically.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/14.

21 Metal-containing organic compounds:

Library under subclass 15 wherein the library members are organic compounds which contain a metal.

- (1) Note. A metal is an element other than hydrogen (H), boron (B), carbon (C), silicon (Si), nitrogen (N), phosphorus (P), oxygen (O), sulfur (S), selenium (Se), tellurium (Te), fluorine (F), chlorine (Cl), bromine (Br), iodine (I), astatine

(At), helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rd).

- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/16.

22 Library containing only inorganic compounds or inorganic materials:

Library under subclass 13 wherein the library members are solely inorganic in nature.

- (1) Note. Inorganic compounds include compounds consisting of only carbon atoms (e.g., fullerenes, etc.), cyanogen, cyanogen halides, cyanamide, metal carbides, hydrocyanic acid, isocyanic acid, isothiocyanic acid, fulminic acid, and salts of the previously mentioned acids. They do not include compounds satisfying one of the following criteria: (a) at least two carbon atoms bonded to each other, or (b) one carbon atom bonded to at least one hydrogen atom or halogen atom, or (c) one carbon atom bonded to at least one nitrogen atom by a single or double bond.

- (2) Note. An inorganic material includes alloys composed of two or more metals which may be (a) chemically united, (b) in the form of a mixture, or (c) in solid solution.

- (3) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 40/18.

SEE OR SEARCH CLASS:

420, Alloys or Metallic Compositions, for alloys, per se, containing metal or metallic compositions which contain a continuous phase of metal and methods of making same not provided for elsewhere. This class will also take elemental metal, per se.

423, Chemistry of Inorganic Compounds, for inorganic compounds, per se, and nonmetallic elements, per se, and processes of producing by a chemical reaction.

23 METHOD OF CREATING A LIBRARY (E.G., COMBINATORIAL SYNTHESIS, ETC.):

This subclass is indented under the class definition. Method which is directed to the preparation of a library, which method may include simple physical admixture of components, synthesis via chemical reaction, synthesis via a biological process (e.g., microbial, enzymatic, etc.), or any other synthetic means.

- (1) Note. Combinatorial synthesis is the preparation of sets of diverse entities by the combination of sets of chemical building blocks (e.g., reagents, etc.).
- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/00.

24 In silico or mathematical conception of a library:

Method under subclass 23 involving preparation of a library in electronic form or on paper to be used in the design and evaluation of potential libraries.

- (1) Note. The building blocks for preparing an in silico library may not exist, and the chemical steps for creating such a library may not have been tested.
- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/02.

25 Using a dynamic combinatorial chemistry technique:

Method under subclass 23 for preparing a library involving a technique in which a target compound is introduced into a mixture of library constituents that are able to interconvert with each other chemically, wherein some of the library constituents bind to the target compound selectively and are therefore removed from the pool of interconverting species, thereby causing the equilibrium of the library solution to shift, favoring the production of species that bind to the target and minimizing the concentration of poorly binding library compounds.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/04.

26 Biochemical method (e.g., using an enzyme or whole viable micro-organism, etc.):

Method under subclass 23 for preparing a library involving the use of enzymes, vectors, micro-organisms, or antibodies.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/06.

27 Liquid-phase synthesis (i.e., wherein all library building blocks are in liquid phase or in solution during library creation) or particular method of cleavage from the liquid support used:

Method under subclass 23 wherein building blocks of a library are in a liquid phase during library creation or a specifically recited method of cleaving the library from the liquid support is used.

- (1) Note. For the purposes of this subclass, liquid-phase synthesis includes both solution-phase synthesis (i.e., synthesis involving only one liquid phase) and multiple liquid-phase synthesis (i.e., synthesis involving more than one liquid phase). The latter synthesis may involve synthesis performed on a liquid macromolecular compound (soluble support) such as polyethylene glycol (PEG), a dendrimers, or wherein a fluorocarbon phase is present in the system (i.e., fluororous synthesis).
- (2) Note. A soluble support is an attachment, common to all library members, which renders the library components soluble under conditions for library synthesis, but which can be readily separated from most other soluble components when desired by some simple physical process.
- (3) Note. Fluororous synthesis is a type of 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 comprising a fluorinated solvent.

- (4) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/08.

28 Involving an encoding step:

Method under subclass 27 wherein the method of preparing a library involves associating a unique tag (chemical or nonchemical) sequentially with each support when each library building block is added, therefore recording a history of building block additions which each support has been subjected to, during the entire synthesis.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/10.

29 Using a particular method of attachment to the liquid support:

Method under subclass 27 wherein a specific method of attachment of the library building blocks focuses on the way the building blocks are bound to the liquid support (e.g., by means of electrostatic interactions, formation of covalent bonds by cycloaddition reactions, irradiation, etc.).

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/12.

30 Solid-phase synthesis (i.e., wherein one or more library building blocks are bound to a solid support during library creation) or particular method of cleavage from the solid support used:

Method under subclass 23 wherein one or more of the building blocks of a library bound to a solid support (e.g., resin bead, etc.) during library creation or a specifically recited method of cleaving the library from the solid support is used.

- (1) Note. A solid support is an insoluble, functionalized, polymeric material to which library members or reagents may be attached (often via a linker) allowing them to be readily separated (by filtration, centrifugation, etc.) from excess

reagents, soluble reaction by-products, or solvents.

- (2) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/14.

31 Involving an encoding step:

Method under subclass 30 wherein the method of preparing a library involves associating a unique tag (chemical or nonchemical) sequentially with each solid support (e.g., bead, etc.) when each library building block is added, therefore recording a history of building block additions which each solid support has been subjected to, during the entire synthesis.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/16.

32 Using a particular method of attachment to the solid support:

Method under subclass 30 wherein a specific method of attachment of the library building blocks focuses on the way the building blocks are bound to the solid support (e.g., by means of electrostatic interactions, formation of covalent bonds by cycloaddition reactions, irradiation, etc.).

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 50/18.

33 APPARATUS SPECIALLY ADAPTED FOR USE IN COMBINATORIAL CHEMISTRY OR WITH A LIBRARY:

This subclass is indented under the class definition. Apparatus which is uniquely designed or specially adapted for use in combinatorial chemistry technology.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/00.

SEE OR SEARCH CLASS:

422, Chemical Apparatus and Process Disinfecting, Deodorizing, Preserving, or Sterilizing, subclasses 50 through 570 for apparatus for performing an analysis which involves a chemical or physical reaction not elsewhere pro-

- vided for and subclasses 129-242 for carrying out chemical reactions.
- 435, Chemistry: Molecular Biology and Microbiology, subclasses 283.1 through 309.4 for apparatus for fermentation, enzymology, organ or tissue maintenance, or genetic engineering.
- 34 Integrated apparatus specially adapted for creating a library, screening a library, and for identifying a library member:**
Apparatus under subclass 33 which is specifically designed for performing the preparation of a library, the screening of library members for certain activities or properties, and the identification of the exact nature of particular library members.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/02.
- 35 Integrated apparatus specially adapted for both screening a library and identifying a library member:**
Apparatus under subclass 33 which is specifically designed for performing the screening of library members for certain activities or properties and the identification of the exact nature of particular library members.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/04.
- 36 Integrated apparatus specially adapted for both creating a library and identifying a library member:**
Apparatus under subclass 33 which is specifically designed for performing the preparation of a library and the identification of the exact nature of particular library members.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/06.
- 37 Integrated apparatus specially adapted for both creating and screening a library:**
Apparatus under subclass 33 which is specifically designed for performing the preparation of a library and the screening of library members for certain activities or properties.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/08.
- 38 For identifying a library member:**
Apparatus under subclass 33 which is specifically designed for performing the identification of the exact nature of particular library members.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/10.
- 39 For screening a library:**
Apparatus under subclass 33 which is specifically designed for performing the screening of library members for certain activities or properties.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/12.
- 40 For creating a library:**
Apparatus under subclass 33 which is specifically designed for performing the preparation of a library.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 60/14.
- 41 TAG OR LABEL SPECIALLY ADAPTED FOR COMBINATORIAL CHEMISTRY OR A LIBRARY (E.G., FLUORESCENT TAG, BAR CODE, ETC.):**
This subclass is indented under the class definition. Subject matter which is a tag or label unique for use in combinatorial chemistry techniques or unique as an identifier of a library or library members.
- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 70/00.
- 42 LINKER OR SPACER SPECIALLY ADAPTED FOR COMBINATORIAL CHEMISTRY OR A LIBRARY (E.G.,**

TRACELESS LINKER, SAFETY-CATCH LINKER, ETC.):

This subclass is indented under the class definition. Subject matter for use in combinatorial chemistry techniques which involves a chemical constituent which is used to connect a compound to a support or another compound in order to enhance a reaction outcome.

- (1) Note. A linker is a bifunctional molecule attaching a compound or first building block of a synthesis to a solid or soluble support which can be cleaved to release compounds from the support.
- (2) Note. A traceless linker is one which does not leave any residue on a compound after cleavage from a support (i.e., linker is replaced by a hydrogen atom).
- (3) Note. A safety-catch linker is cleaved by performing two different reactions instead of only one, thus providing greater control over the timing of compound release. For example, a sulfonamide resin is "activated" before the actual cleavage takes place (e.g., cleavage by nucleophilic displacement of a previously alkylated sulfonamide resin).
- (4) Note. A spacer is a chemical moiety used in solid-phase synthesis to influence reaction conditions, reduce steric hindrance, modify hydrophobicity, etc.
- (5) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 80/00.

43 MISCELLANEOUS:

This subclass is indented under the class definition. Subject matter which is not provided for in other subclasses.

- (1) Note. The subject matter in this subclass is substantially the same in scope as IPC C40B 99/00

END