(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
14 June 2018 (14.06.2018)

WIPO | PCT

(10) International Publication Number
WO 2018/103642 A1

(51) International Patent Classification:
G06F 17/30 (2006.01)

(21) International Application Number:
PCT/CN2017/114656

(22) International Filing Date:
05 December 2017 (05.12.2017)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
62/430,289 05 December 2016 (05.12.2016) US

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(54) **Title:** SYSTEMS, APPARATUSES, AND METHODS FOR SEARCHING AND DISPLAYING INFORMATION AVAILABLE IN LARGE DATABASES ACCORDING TO THE SIMILARITY OF CHEMICAL STRUCTURES DISCUSSED IN THEM

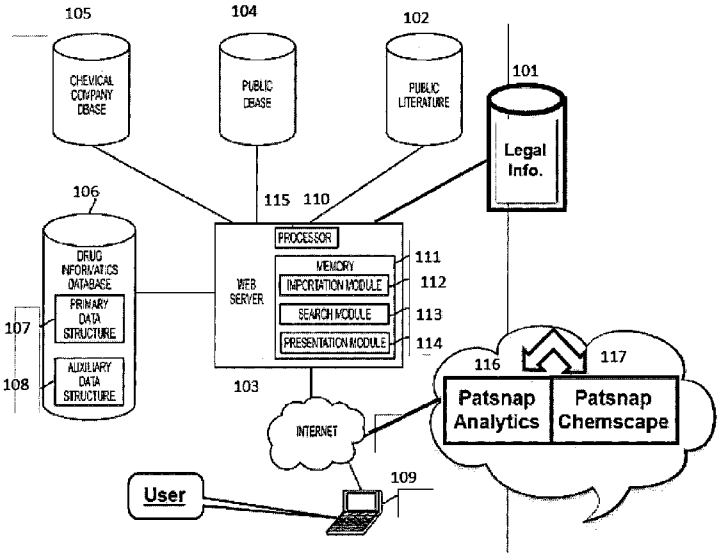

Fig. 1

(57) **Abstract:** Systems, methods, and apparatuses for improving a search for chemical structure content in an information space within and across patents and other literature available in a wide range of databases, and it incorporates a new tool for visualizing chemical space in landscape formats. More particularly, systems, methods, and apparatuses for using public information available from a variety of databases and Internet-based resources to obtain and group information to determine similar chemical structures, undertake three-dimensional landscape analyses to access those similar structures and obtain other information about them including but not limited to patent data, patent family structures, litigation-related information, regulatory and marketing approval information, and other types of information that helps a user understand the medical, technical, and legal landscape associated with certain chemical structures of

[Continued on next page]

WO 2018/103642 A1

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(81) **Designated States** *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) **Designated States** *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

Published:

— *with international search report (Art. 21(3))*

interest as well as related chemical structures. In addition, the embodiments provide a novel navigation paradigm of search results and content items so that the user can more intuitively and more efficiently get and manipulate information relating to chemical structures that are grouped based on their chemical similarities.

SYSTEMS, APPARATUSES, AND METHODS FOR SEARCHING AND DISPLAYING INFORMATION AVAILABLE IN LARGE DATABASES ACCORDING TO THE SIMILARITY OF CHEMICAL STRUCTURES DISCUSSED IN THEM

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application No. 62/430,289, entitled "Searching and Displaying Documents in Large Databases According to the Similarity of Chemical Structures Discussed in Them," filed December 5, 2016. This application is incorporated by reference in its entirety.

FIELD OF THE INVENTION

Embodiments of the present invention relate to systems, methods, and apparatuses for improving a search for chemical structure content in an information space within and across patents and other literature available in a wide range of databases, and it incorporates a new tool for visualizing chemical space in landscape formats. More particularly, embodiments of the present invention relate to systems, methods, and apparatuses for using public information available from a variety of databases and Internet-based resources to obtain and group information to determine similar chemical structures, undertake three-dimensional landscape analyses to access those similar structures and obtain other information about them including but not limited to patent data, patent family structures, litigation-related information, regulatory and marketing approval information, and other types of information that helps a user understand the medical, technical, and legal landscape associated with certain chemical structures of interest as well as related chemical structures.

BACKGROUND

Information spaces, such as the Internet, enterprise networks, document repositories, and information storage and retrieval services allow for widespread access to large collections of information. For example, users commonly use Internet search engines to locate and select desired information on the Internet or within public or proprietary

databases relating to products, individual patents and their associated data, simple and complex patent family information, regulatory activity associated with products covered by patents such as FDA approvals, extensions, adjustment, and reductions of patent terms, court and agency activities affecting patent rights and the appropriate interpretation of certain patent claim terms, and medical information associated with certain chemicals including active pharmaceutical ingredients (APIs) found in drug products subject to regulatory oversight and approval. A wide variety of users performing searches relating to chemical structures and patents have an interest in understanding a number of factors and pieces of data that relate to those structures and analyzing and ultimately prioritizing many pieces of information that reside in information silos and discrete databases that are most relevant to their search.

While a manual search and comparison of such information can provide some useful information to a user, the current tools do not provide a system, method or apparatus that gives real-time updates and chemical structure groupings to the user involving similar chemical structures and visualization of chemical spaces.

Search engines assist users in locating items in an information space. Such items can include documents, images, videos, and many other kinds of files known in the art. The search engines typically use search algorithms that employ either literal keyword matching techniques or approximate matching of the words or symbols specified in a user's query or search request. Thus, in conventional searches in discrete data sets and databases, a user searching for information must provide keywords that will hopefully match the desired content. In practice, however, this methodology is little more than a guessing game for both content users and content providers and is particularly difficult when the searches relate to chemical structures. A variety of keywords can be used to conceptual ideas, which can make tagging and keyword searching difficult. In addition, a given combination of keywords is unlikely to be the same between systems providing information regarding particular chemical structures. Accordingly, concept matching or semantic matching of chemical structures and information associated with those structures within search engines can be poor and inconsistent. Conventional search and analysis tools can also be ineffective at ascertaining meaning that is inherent in chemical structures. For many

systems, content is expressed in natural language with no convention or chemical structure organization governing the meaning or clustering of the content. Thus, search engines are, in general, unable to locate or group the most appropriate or relevant chemical structure content reliably. It is not currently feasible to rely on the current search tools to group or organize chemical structure content based on the similarity of those structures.

While systems and algorithms that group data based on various pre-defined text parameters are known, they are not useful to relate and correlate information relating to two and three dimensional chemical structures and their associated chemical compound names, including the nomenclature developed by the International Union of Pure and Applied Chemistry (IUPAC); the International Chemical Identifier (InChi) system, which reflects a compound's structure and composition; as well as CAS numbers, which each refer to a single compound and do not contain any information about the structure.

Managing and mapping patent related information in general is known and reference is made to US 9607058 to Gupta and US 96975 to Lundberg. Despite some benefits provided by prior art techniques; these tools nevertheless fall short of providing meaningful groupings of chemical structures and other information that is relevant to those chemical structures, including patent information, to provide users actionable insights regarding certain chemical structures of interest.

SUMMARY OF THE INVENTION

This summary is provided to introduce certain concepts in a simplified form that are further described below in the Detailed Description and Drawings. This summary is not intended to identify key features or essential features of the claimed subject matter, nor is it intended to limit in any way the scope of the claimed invention.

The new PatSnap software platform, based around chemical structure searching within and across patents and other literature, incorporates a new tool for visualizing chemical space. This chemical landscaping tool, also called 'Chemscape', is a analytic system, method and apparatus, which arranges chemical structures as squares across a 2D plane based on similarities in their structure. Chemical structures that are most similar to each other are found closer to one another. The bigger a change in chemical structure, the more

distant they are from one another. This calculation is multiplied across thousands of structures to give a graphical representation of how a selection of structures can be gathered into groups.

Clicking on these representative squares reflecting groupings of similar chemical structures will open up a tool displaying the structure, describing its properties, and providing information on and linking to a wide variety of public material (and some material only available on proprietary databases) including scientific literature, patent materials including patent family information, medical and regulatory information, henceforth collectively referred to as 'literature', that mentions any of the chosen structures of interest.

A 3D layer is then added, which involves the arranged squares (representing the chemical structures), being represented as 3D columns within the tool. In one example, the height of the column is representative of the number of individual 'literature' papers that mention the corresponding chemical structure. In another example, the height of the column is representative of the number of data sources involving the corresponding structure. In another example, the height of the column is representative of the proteins or other chemical entities that corresponding structure is grouped with due to the their chemical structure similarities.

This 'Chemscape' tool can, in an optional embodiment, be animated to give a dynamic overview of how 'literature' mentioning the corresponding chemical structures have been published over time. This includes 3D columns that reflect the publication dates of the 'literature' mentioning the structures, and the columns increase in height as a timeline increases in length.

The 2D squares and 3D columns can, in an optional embodiment, be highlighted based on information relating to the underlying chemical structures associated with the data set, such as structural similarity scores in reference to a query structure, regulatory approval information, clinical trial phases, statuses, and sources of the corresponding chemical structure information. These squares and columns can also, in another optional embodiment, be highlighted based on information relating to the patents or literature

mentioning the chemical structures, such as patent classification codes, publication dates, patent filing or expiration dates, assignees, normalized assignees, inventors on patents, and scientific references mentioning the chemical structure.

On top of this chemical structure and associated information visualization tool, is the ability to search across literature (including associated patents and scientific references) based on keyword searching within 'literature' text, or information searching across 'literature' metadata. Upon inputting a search query, the 3D columns change, in an optional embodiment, in height based on refinement of the corresponding 'literature' to reflect the number of refined 'literature' results that mention the chemical structure and qualify the results based on the user-inputted query refinement information.

The present system, method, and apparatus provides a novel two-dimensional matrix reflecting a grouping of chemical structures based on the similarity of their chemical structures and associated literature that the user can analyze along with the grouped chemical structures to better understand the legal, regulatory, and medical status of them.

BRIEF DESCRIPTION OF THE DRAWINGS

The present invention will now be described more fully hereinafter with reference to the accompanying drawings, which illustrate various embodiments of the invention. This invention, however, may be embodied in many different forms and should not be construed as limited to the embodiments set forth herein. Rather, these embodiments are provided so that this disclosure will be thorough and complete, and will fully convey the scope of the invention to those skilled in the art. It is to be fully recognized that the different teachings of the various embodiments discussed below may be employed separately or in any suitable combination to produce desired results. The various characteristics mentioned above, as well as other features and characteristics described in more detail below, will be readily apparent to those skilled in the art upon reading the following detailed description of the various embodiments, and by referring to the accompanying drawings. In the drawings and description that follow, like parts are marked throughout the specification and drawings with the same reference numerals, respectively. The prime notation, if used, indicates similar elements in alternative embodiments. The drawings are not necessarily to

scale. Certain features of the disclosure may be shown exaggerated in scale or in somewhat schematic form and some details of conventional elements may not be shown in the interest of clarity and conciseness.

Figure 1 is a schematic block diagram of an exemplary method according to an embodiment of the invention. Figure 2 is a representative excerpt of a patent application accessible through an exemplary method according to an embodiment of the invention.

Figure 3 is a representative excerpt of a court filing accessible through an exemplary method according to an embodiment of the invention.

Figure 4 is a representative excerpt of Food and Drug Administration (FDA) correspondence accessible through an exemplary method according to an embodiment of the invention.

Figure 5 is a representative excerpt of public information regarding drug exclusivity expiration dates accessible through an exemplary method according to an embodiment of the invention.

Figure 6 is a screenshot of public information reflecting regulatory approval and drug exclusivity information accessible through an exemplary method according to an embodiment of the invention.

Figure 7 is a screenshot of the Patsnap chemical tool search page according to an embodiment of the invention.

Figure 8 is a screenshot excerpt of an exemplary search performed according to an embodiment of the invention.

Figure 9 is a screenshot excerpt of sample patent and associated patent information accessible through an exemplary method according to an embodiment of the invention.

Figure 10 is a screenshot excerpt of sample legal information associated with a sample patent accessible through an exemplary method according to an embodiment of the invention.

Figure 11 is a screenshot excerpt of patent map associated with a patent family accessible through an exemplary method according to an embodiment of the invention.

Figure 12 is a simple patent family and patent citation map compiled through an exemplary method according to an embodiment of the invention.

Figure 13 is a representative excerpt of chemical structure information accessible through an exemplary method according to an embodiment of the invention.

Figure 14 is a screenshot excerpt of a chemical structure search that can be performed through an exemplary method according to an embodiment of the invention.

Figure 15 is a screenshot excerpt of a chemical structure reflecting the search that was performed in figure 14.

Figure 16 is a screenshot excerpt reflecting information regarding the chemical structure search that was performed in figure 14.

Figure 17 is a screenshot excerpt reflecting analytical tools relating to the chemical structure reflected in figure 15.

Figure 18 is a screenshot excerpt reflecting the search performed using the analytical tools reflected in figure 17.

Figure 19 is a screenshot excerpt reflecting chemical structures deemed similar to the chemical structure reflected in the search performed in figure 14.

Figure 20 is a screenshot excerpt reflecting a patent literature search with the chemical structure reflected in figure 16.

Figure 21 is a screenshot excerpt reflecting the results of the patent literature search in figure 20.

Figure 22 is a representative excerpt of chemical structure information accessible through an exemplary method according to an embodiment of the invention.

Figure 23 is a screenshot excerpt reflecting various analytical tools and data summaries accessible through an exemplary method according to an embodiment of the invention.

Figure 24 is a screenshot excerpt reflecting a three dimensional model of chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 25 is a screenshot excerpt reflecting an analytical tool regarding analysis of chemical structures reflected in a three-dimensional model accessible through an exemplary method according to an embodiment of the invention.

Figure 26 is a screenshot excerpt reflecting a two-dimensional model of chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 27 is a screenshot excerpt reflecting an analytical tool relating to analysis of a collection of similar chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 28 is a screenshot excerpt reflecting a listing of grouped chemical structures and associated patent and chemical structure information relating to analysis of a collection of similar chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 29 is a screenshot excerpt reflecting patent related information associated with a group of chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 30 is a screenshot excerpt reflecting a three-dimensional model of chemical structures and associated chemical structure identification information accessible through an exemplary method according to an embodiment of the invention.

Figure 31 is a screenshot excerpt reflecting a three-dimensional model of chemical structures and associated chemical structure identification and patent information accessible through an exemplary method according to an embodiment of the invention.

Figure 32 is a screenshot excerpt reflecting a three-dimensional model of chemical structures reflecting a listing of grouped chemical structures and associated chemical

structure identification and patent information accessible through an exemplary method according to an embodiment of the invention.

Figure 33 is a screenshot excerpt reflecting patent grouping information, regulatory approval information, and patent classification information accessible through an exemplary method according to an embodiment of the invention.

Figure 34 is a screenshot excerpt reflecting a three-dimensional model of chemical research structures reflecting a listing of international classification groups for related chemical structures accessible through an exemplary method according to an embodiment of the invention.

Figure 35 is a screenshot excerpt reflecting a three-dimensional model of chemical structures and a patent search menu accessible through an exemplary method according to an embodiment of the invention.

Figure 36 is a screenshot excerpt reflecting the results of a patent search result accessible through an exemplary method according to an embodiment of the invention.

Figure 37 is a chart reflecting various exemplary search operations and methodologies that can be used with an exemplary method according to an embodiment of the invention.

Figure 38 is a screenshot excerpt reflecting a structure editor accessible through an exemplary method according to an embodiment of the invention.

Figure 39 is a screenshot excerpt reflecting a structure editor and an additional structure analysis tools accessible through an exemplary method according to an embodiment of the invention.

Figure 40 is a schematic diagram of an exemplary method of practicing searches and analyses involving chemical structures utilizing an apparatus according to an embodiment of the present invention.

Figure 41 is a schematic diagram of an exemplary method of practicing searches and analyses involving chemical structures utilizing an apparatus according to an embodiment of the present invention.

Figure 42 is a schematic diagram of an exemplary method of practicing searches and analyses involving chemical structures and using the three-dimensional visualization tools according to an embodiment of the present invention.

Figure 43 is a diagram of an exemplary output as a result of practicing searches and analyses involving chemical structures using the three-dimensional visualization tools according to an embodiment of the present invention.

Figure 44 is a diagram reflecting exemplary data sources and data sets searched and analyzed according to an embodiment of the present invention.

Figure 45 is a diagram reflecting an exemplary system and set of components used to process and output the results of searches and analyses involving chemical structures using the two-dimensional or three-dimensional visualization tools according to an embodiment of the present invention.

DESCRIPTION OF THE EMBODIMENTS

Embodiments of the present invention are described in the accompanying drawings, wherein like parts are designated by like reference numerals throughout, and wherein the leftmost digit of each reference number refers to the drawing number of the figure in which the referenced part first appears.

The invention includes a method for visually mapping chemical structures based on their structural similarities and associating a wide variety of literature relating to said chemical structures comprising maintaining a system with at least one database of chemical structures and at least one database of public literature, wherein said public literature includes information regarding chemical structures; receiving from a requesting user a request for information on a target chemical structure provided by the requesting user from a user interface generated on a display by at least one computer processor; in response to the request for information on a target chemical structure, providing a set of related chemical structures to the requesting user, based on the chemical similarity of the plurality of related chemical structures provided to the target chemical structure; wherein said at least one database of chemical structures is stored on at least one storage device;

wherein said at least one database of public literature is stored on at least one storage device.

In general, embodiments of the present invention provide a novel approach for more efficient searching, knowledge discovery, content discovery, and browsing or navigating in an information space to review and associate chemical structures and literature information. In some embodiments, systems and methods provide a2D and 3D oriented structure for organizing and accessing information associated with chemical structures. Optional embodiments of the present invention leverage the semantics of literature, shape of the chemical structures, fingerprinting, or Tanimoto scoring and the goal of a user's search to provide a novel two and three dimensional navigation paradigm of search results and content items so the user can more intuitively and more efficiently get access to and analyze information related to chemical structures housed within at least one database of chemical structures.

In some embodiments, a user can navigate or descend through various levels or nodes of literature related to chemical structures. This information can be presented in any type of two dimensional or three-dimensional data structure or graph, as well as hierarchical or non-hierarchical outputs. The information outputs may be structured to provide a progressively narrower scope of subject matter related to a chemical structure, which can help users to search and/or browse for content of a specific type or semantic context and then drill down on certain content of interest using a visual representation of that information.

A content source can be any body of information, including databases having individual items of content. An example of such a content source is the World Wide Web, where content item can be a resource accessible via a uniform resource locator ("URL") on the Internet. Content items may also include URLs that correspond to web pages, images, files, or other items that can be provided to a user, such as via a browser or other type of content interface applications.

In some embodiments, the semantic meaning of content items can be based on interpretations of interactions users take to organize and review the content items within

an organized content structure. The semantics of content items may also be determined based on a user's declarations or inputs in the database about the content items.

Some embodiments are based on systems and methods for determining the relationship of content items as indicated by user-derived information. User-derived information may be any information that originates from an individual user, including the user requesting the search, a group of users, or an entire community of users. That is, the embodiments provide mechanisms and techniques for improving and capturing relationships between literature and chemical structures as the information is organized by users in a user community, based on, among other things, user interactions with the information in at least one database. Accordingly, some embodiments provide an organized report of related chemical structures, so that users can search for target chemical structures, navigate or browse chemical structures, organize literature information, and perform other operations on information within that report of chemical structures. Any of those operations can indicate importance of the literature related to chemical structures. User-derived information can be anonymous or identified with one or more users or user groups.

In some embodiments, a user can navigate through a tool that provides organized content structure to discover and view target chemical structures and related chemical structures. The organization and grouping of the chemical structures and related literature information that are provided to users through a two-dimensional or three-dimensional report can provide valuable contextual information that allows the user to take some action with respect to the target chemical structure.

An organized content structure may be implemented in various ways, including providing visual reports that incorporate several different kinds of folders, trees, lists, graphs, databases, and/or other appropriate data structures known in the art. An organized content structure may be delivered locally for access by a single user through a display on a local computer or saved within a platform for simultaneous access by many users. Global implementations can include cloud-based systems known in the art or distributed systems where portions of the organized content structure may exist on a plurality of computing systems. The storage for a local organized content structure may be

implemented physically on a user's own client device, such as a hard disk drive, or implemented virtually using remote services over a network, such as cloud-based storage. In addition, a local organized content structure may comprise a similar semantic organization as a global organized content structure, but the local organized content structure may content items that are retained for the specific purposes of a user.

Embodiments of the present invention can apply to repositories of literature that are small or moderate in size, as well as the largest distributed repositories of literature, such as databases that retain and index documents obtained from web crawlers, etc. operating on the World Wide Web. Embodiments of the invention provide the user with a more controlled and interactive approach to locating literature relating to chemical structures. The embodiments provide various modalities of searching for literature using queries and navigating an organized structure, such as a hierarchy of interactive menus or folders in a user interface, alone or in combination.

Overview of the Chemscape Tool

Embodiments of the invention can provide a search engine configured to generate an output of chemical structures that are grouped based on their structural similarities, as well as additional literature that relates in some manner to one or more of those chemical structures, for a particular user for the purpose of providing a variety of information relating to those structures including medical data, regulatory approvals, legal information (including patent information). That is, a user can ask for literature information relating to a known chemical structure or related chemical structures and navigate that information using two and three dimensional visualization tools. In response to user activities, the Chemscape tool may search a collection of databases, and based on a variety of known search techniques further discussed below, the tool may identify additional literature or chemical structures that are related to or similar to the known chemical structure and its associated literature. The determination of chemical structure similarity can be optionally made based on actions that other users have taken within the organized content structure to organize and associate any of the known set of documents with other content items.

Embodiments of the invention are directed to systems, methods, and apparatuses for providing similar chemical structures and associated literature in this fashion, using association criteria as discussed in the example above, as well as more complex relational criteria as described below.

The invention also includes a method of automatically computing, mapping and accessing chemical structure similarities in conjunction with corresponding non-chemical (patent, legal and medical data) records comprising: (a) Selecting/entering a target chemical structure from a data base using a User Interface generated on a display by a processor of a computer system, where the user interface being associated to a patent-related search engine linked to the data base, the search engine and the data base being hosted in either a first memory of the computer system or in a remotely located second memory; and (b) Obtaining from the data base chemical structure records related to the target chemical structure to create via the processor a 2D-map from a user-input method and from a first data sets of chemical records stored in the first memory or the second memory.

The Chemscape tool is based around chemical structure searching within and across patents and other literature, incorporates a new tool for visualizing chemical space. This chemical landscaping tool is an analytic system, method and apparatus, which arranges chemical structures as squares across a 2D plane based on similarities in their structure. Chemical structures that are most similar to each other are found closer to one another. The bigger a change in chemical structure, the more distant they are from one another. This calculation is multiplied across thousands of structures to give a graphical representation of how a selection of structures can be gathered into groups.

Clicking on these representative squares reflecting groupings of similar chemical structures will open up a tool displaying the structure, describing its properties, and providing information on and linking to a wide variety of public material (and some material only available on proprietary databases) including scientific literature, patent materials including patent family information, medical and regulatory information, henceforth collectively referred to as 'literature', that mentions any of the chosen structures of interest.

A 3D layer is then added, which involves the arranged squares (representing the chemical structures), being represented as 3D columns within the tool. In one example, the height of the column is representative of the number of individual 'literature' papers that mention the corresponding chemical structure. In another example, the height of the column is representative of the number of data sources involving the corresponding structure. In another example, the height of the column is representative of the proteins or other chemical entities that corresponding structure is grouped with due to the their chemical structure similarities.

This 'Chemscape' tool can be animated to give a dynamic overview of how 'literature' mentioning the corresponding chemical structures have been published over time. This includes 3D columns that reflect the publication dates of the 'literature' mentioning the structures, and the columns increase in height as a timeline increases in length.

The 2D squares and 3D columns can, in an optional embodiment, be highlighted based on information relating to the underlying chemical structures associated with the data set, such as structural similarity scores in reference to a query structure, regulatory approval information, clinical trial phases, statuses, and sources of the corresponding chemical structure information. These squares and columns can also, in another optional embodiment, be highlighted based on information relating to the patents or literature mentioning the chemical structures, such as patent classification codes, publication dates, patent filing or expiration dates, assignees, normalized assignees, inventors on patents, and scientific references mentioning the chemical structure.

On top of this chemical structure and associated information visualization tool, is the ability to search across literature (including associated patents and scientific references) based on keyword searching within 'literature' text, or information searching across 'literature' metadata. Upon inputting a search query, the 3D columns change, in an optional embodiment, in height based on refinement of the corresponding 'literature' to reflect the number of refined 'literature' results that mention the chemical structure and qualify the results based on the user-inputted query refinement information.

The present system, method, and apparatus provides a novel two-dimensional matrix reflecting a grouping of chemical structures based on the similarity of their chemical structures and associated literature that the user can analyze along with the grouped chemical structures to better understand the legal, regulatory, and medical status of them.

In optional embodiments, the selecting occurs via a menu/or automation function activated via the processor using a first method to determine a first set of molecular similarities with respect to the target chemical structure, where the method includes at least a Tanimoto Scoring and Fingerprinting, a Semantic similarity, or a Shape similarity among the chemical structures.

In optional embodiments, the generating occurs via the processor to provide a first non-linear clustering map of similar chemical structure records using the selected similarity determination method.

Additionally, the results are displayed optionally on a computer screen and reflect the first non-linear clustering of the chemical structures records on a plane as a 2d-map according to a 1st graphic distribution method of the similar chemical structures.

In other embodiments, the results obtained involve a single or a plurality of user-selected non-chemical secondary data set records from a source/library hosted in the first or second memory and linked to the 2d-map of chemical structure similar records.

The tool may also optionally arrange and display the selectable secondary data set records related to the 2D-map chemical structures as a 3D- map of graphic elements to simultaneously and visually link-associate the non-chemical secondary data set records to the 2D-map of chemical structures. The tool may further display the secondary data set records according to a particular and selectable task without exiting the search engine to access and visualize the secondary data set records. The records may be displayed as 3D cuboidal, cylindrical, or other shaped bar, with height of 3D bar representing the count of secondary data records.

The user may also access the secondary non-chemical data set records linked to the chemical records of the 2D-map via the 3D-map by clicking on one or several select graphic element via an inputting or a pointing device.

Literature Available to Chemscape Tool

Search results provided by embodiments of the present invention may operate on the following data objects, databases, or information entities, though these lists are not intended to be limiting as other similar data items may also be included:

1) As mentioned above, content items (sometimes referred to as "content," or "items") are discrete information resources. Content items can be, for example, web pages or other components of web pages that can be specified and stored as a reference (for example, by a Uniform Resource Locator, or "URL"). Content items can also be videos, sound files, images, and documents of all kinds, including PDF files, word processing files (e.g., Microsoft Word), spreadsheets (e.g., Microsoft Excel), presentation files (e.g., Microsoft PowerPoint), graphics files, source code files, executable files, databases, messages, configuration files, data files, and the like. Content items can be accessed, reviewed, modified, and saved by users of systems implemented by any of the embodiments.

2) Databases that include information relating to patent applications, published patents, granted patents, patent families, patent terminal disclaimers, legal decisions and opinions relating to patent validity or infringement, interpretation of patent claim terms, patent term adjustments and extensions, regulatory activities relating to patents (including adjustment of patent terms for delay due to regulatory approval, orphan drugs, and new approved uses) and medical information relating to adverse events, approved uses and treatments, as well as medical and scientific literature databases.

Embodiments of the System

The system of the present invention may comprise any device and/or means for rendering information to a user and/or requesting information from the user. A user interface includes at least one of textual, graphical, audio, video, animation, and/or haptic elements. A textual element can be provided, for example, by a printer, monitor, display, projector, etc. A graphical element can be provided, for example, via a monitor, display, projector, and/or visual indication device, such as a light, flag, beacon, etc. An audio element can be provided, for example, via a speaker, microphone, and/or other sound

generating and/or receiving device. A video element or animation element can be provided, for example, via a monitor, display, projector, and/or other visual device.

A user interface can include one or more textual elements such as, for example, one or more letters, number, symbols, etc. A user interface can include one or more graphical elements such as, for example, an image, photograph, drawing, icon, window, title bar, panel, sheet, tab, drawer, matrix, table, form, calendar, outline view, frame, dialog box, static text, text box, list, pick list, pop-up list, pull-down list, menu, tool bar, dock, check box, radio button, hyperlink, browser, button, control, palette, preview panel, color wheel, dial, slider, scroll bar, cursor, status bar, stepper, and/or progress indicator, etc. A textual and/or graphical element can be used for selecting, programming, adjusting, changing, specifying, etc. an appearance, background color, background style, border style, border thickness, foreground color, font, font style, font size, alignment, line spacing, indent, maximum data length, validation, query, cursor type, pointer type, auto-sizing, position, and/or dimension, etc. A user interface can include one or more audio elements such as, for example, a volume control, pitch control, speed control, voice selector, and/or one or more elements for controlling audio play, speed, pause, fast forward, reverse, etc. A user interface can include one or more video elements such as, for example, elements controlling video play, speed, pause, fast forward, reverse, zoom-in, zoom-out, rotate, and/or tilt, etc. A user interface can include one or more animation elements such as, for example, elements controlling animation play, pause, fast forward, reverse, zoom-in, zoom-out, rotate, tilt, color, intensity, speed, frequency, appearance, etc. A user interface can include one or more haptic elements such as, for example, elements utilizing tactile stimulus, force, pressure, vibration, motion, displacement, temperature, etc.

The present invention can be realized in hardware, software, or a combination of hardware and software. The invention can be realized in a centralized fashion in one computer system, or in a distributed fashion where different elements are spread across several interconnected computer systems. Any kind of computer system or other apparatus adapted for carrying out the methods described herein is suitable. A typical combination of hardware and software can be a general-purpose computer system with a computer

program that, when being loaded and executed, controls the computer system such that it carries out the methods described herein.

Methods of Use

The story of the pharmaceutical drug ZETIA and the need to use the Chemscape tool to a) find similar chemical structure to develop new drugs, b) use data from patents and medical records to assist the researchers in develop new drugs and to avoid litigation demonstrate the novelty and uniqueness of the present invention.

Medical related patents represent an important business tool to promote innovation by securing companies a way to protect their investment in new and useful discoveries. Also such companies can have access, via patent licensing negotiations, to other useful developments coming from a third party's patents of interest.

Patents granted for and related to medical drugs face a tougher challenge considering the FDA regulations and also the continuous legal disputes between the so called medical Brand companies (BC) and Generic companies.

As it is well known, once the life of patent developed by a Brand like company approaches expiration, the Generic like companies will be already ready to manufacture and sell an identical medical drug described and claimed in that patent.

As it is well known, once a patent application filed by a Brand like company (BLC) is published, other Brand like companies or Generic like company will try to "design around" the patents, or develop new drugs by finding "similar chemical structures", or try to patent these new drugs and avoid such publications as prior art.

The patent literature and the non patent literature related to medical drugs is very extensive and the amount of new data and literature will only grow in the future.

There is a need for an increased accuracy and speed to determine via a tool like Chemscape similarities between chemical structures in order to develop new medical drugs and identify a variety of risks associated with the pursuit of various chemical structures as potential active pharmaceutical ingredients in future development efforts.

If a new chemical structure is discovered or a known chemical structure needs to be used in new drugs, there is a need for a tool to collect, process and display automatically all the related chemical data, the patent and the medical data in a manner that meet all the research, patent, legal, medical etc. standards and rules.

Unlike in any other field, the development of a new drug needs to follow many regulations and most important, needs to avoid patent litigation.

Although the present disclosure provides certain embodiments and applications, other embodiments that are apparent to those of ordinary skill in the art, including embodiments, which do not provide all of the features and advantages set forth herein, are also within the scope of this disclosure.

The present invention, as already noted, can be embedded in a computer program product, such as a computer-readable storage medium or device which when loaded in a computer system is able to carry out the different methods described herein. Computer program in the present context means any expression, in any language, code or notation, of a set of instructions intended to cause a system having an information processing capability to perform a particular function either directly or after either or both of the following: a) conversion to another language, code or notation; b) reproduction in a different material form.

The foregoing disclosure has been set forth merely to illustrate the invention and is not intended to be limiting. It will be appreciated that modifications, variations and additional embodiments are covered by the above teachings and within the purview of the appended claims without departing from the spirit and intended scope of the invention. Other logic may also be provided as part of the exemplary embodiments but are left out here so as not to obfuscate the present invention. Since modifications of the disclosed embodiments incorporating the spirit and substance of the invention may occur to persons skilled in the art, the invention should be construed to include everything within the scope of the appended claims and equivalents thereof.

The following examples pertain to further embodiments. Specifics in the examples may be used anywhere in one or more embodiments.

Example 1 is a method of automatically computing, mapping and accessing chemical structure similarities in conjunction with corresponding non-chemical (patent, legal and medical data) records comprising: a) Selecting/entering a target chemical structure from a data base using a User Interface generated on a display by a processor of a computer system, where the user interface being associated to a patent-related search engine linked to the data base, the search engine and the data base being hosted in either a first memory of the computer system or in a remotely located second memory; and b) Obtaining from the data base chemical structure records related to the target chemical structure to create via the processor a 2D-map from a user-input method and from a first data sets of chemical records stored in the first memory or the second memory.

Example 2 is a method of automatically computing, mapping and accessing chemical structure similarities in conjunction with corresponding non-chemical data including patent, legal and medical records, the method comprising: a) Selecting/entering a target chemical structure from a data base using a User Interface generated on a display by a processor of a computer system, where the user interface being associated to a patents' related search engine linked to the data base, the search engine and the data base being hosted in either a first memory of the computer system or in a remotely located second memory; b) Obtaining from the data base chemical structure records related to the target chemical structure to create via the processor a 2D-map from a user-input method and from a first data sets of chemical records stored in the first memory or the second memory; c) Selecting via a menu/or automation function activated via the processor a first method to calculate or evaluate a first set of molecular similarities with respect to the target chemical structure, where the method including at least one of a Tanimoto Scoring and Fingerprinting, a Semantic similarity or a Shape similarity; d) Generating via the processor a first non-linear clustering map of similar chemical structure records using the selected similarity method. e) Displaying on a computer screen the first non-linear clustering of the chemical structures records on a plane as 2d-map according to a 1st graphic distribution method of the similar chemical structures. f) Obtaining a single or a plurality of user-selected non-chemical secondary data set records from a source/library hosted in the first or second memory and linked to the 2d-map of chemical structure similar records. g)

Arranging and displaying the selectable secondary data set records related to the 2D-map chemical structures as a 3D- map of graphic elements to simultaneously and visually link-associate the non-chemical secondary data set records to the 2D-map of chemical structures. h) Accessing the secondary non-chemical data set records linked to the chemical records of the 2D-map via the 3D-map by clicking on one or several select graphic element via an inputting or a pointing device.

Example 3 includes a method of automatically computing, mapping and accessing chemical structure similarities of example 2, further including the step of displaying the secondary data set records according to a particular and selectable task without exiting the search engine to access and visualize the secondary data set records.

Example 4 includes a method of automatically computing, mapping and accessing chemical structure similarities of example 2, further including repeating step (c) by changing the method to evaluate a molecular similarity/dissimilarity.

Example 5 is a method of automatically computing, mapping and accessing chemical structure similarities where the 3D map is used to open and visualize simultaneously the chemical info and at least partially the non-chemical data including.

CLAIMS

The invention claimed is:

1. A method of automatically computing, mapping and accessing chemical structure similarities in conjunction with corresponding non-chemical data including patent, legal and medical records, the method comprising:

a) Selecting/entering a target chemical structure from a data base using a User Interface generated on a display by a processor of a computer system, where the user interface being associated to a patents' related search engine linked to the data base, the search engine and the data base being hosted in either a first memory of the computer system or in a remotely located second memory;

b) Obtaining from the data base chemical structure records related to the target chemical structure to create via the processor a 2D-map from a user-input method and from a first data sets of chemical records stored in the first memory or the second memory;

c) Selecting via a menu/or automation function activated via the processor a first method to calculate or evaluate a first set of molecular similarities with respect to the target chemical structure, where the method including at least one of a Tanimoto Scoring and Fingerprinting, a Semantic similarity or a Shape similarity;

d) Generating via the processor a first non-linear clustering map of similar chemical structure records using the selected similarity method.

e) Displaying on a computer screen the first non-linear clustering of the chemical structures records on a plane as 2d-map according to a 1st graphic distribution method of the similar chemical structures.

f) Obtaining a single or a plurality of user-selected non-chemical secondary data set records from a source/library hosted in the first or second memory and linked to the 2d-map of chemical structure similar records.

g) Arranging and displaying the selectable secondary data set records related to the 2D-map chemical structures as a 3D- map of graphic elements to simultaneously and visually link-associate the non-chemical secondary data set records to the 2D-map of chemical structures.

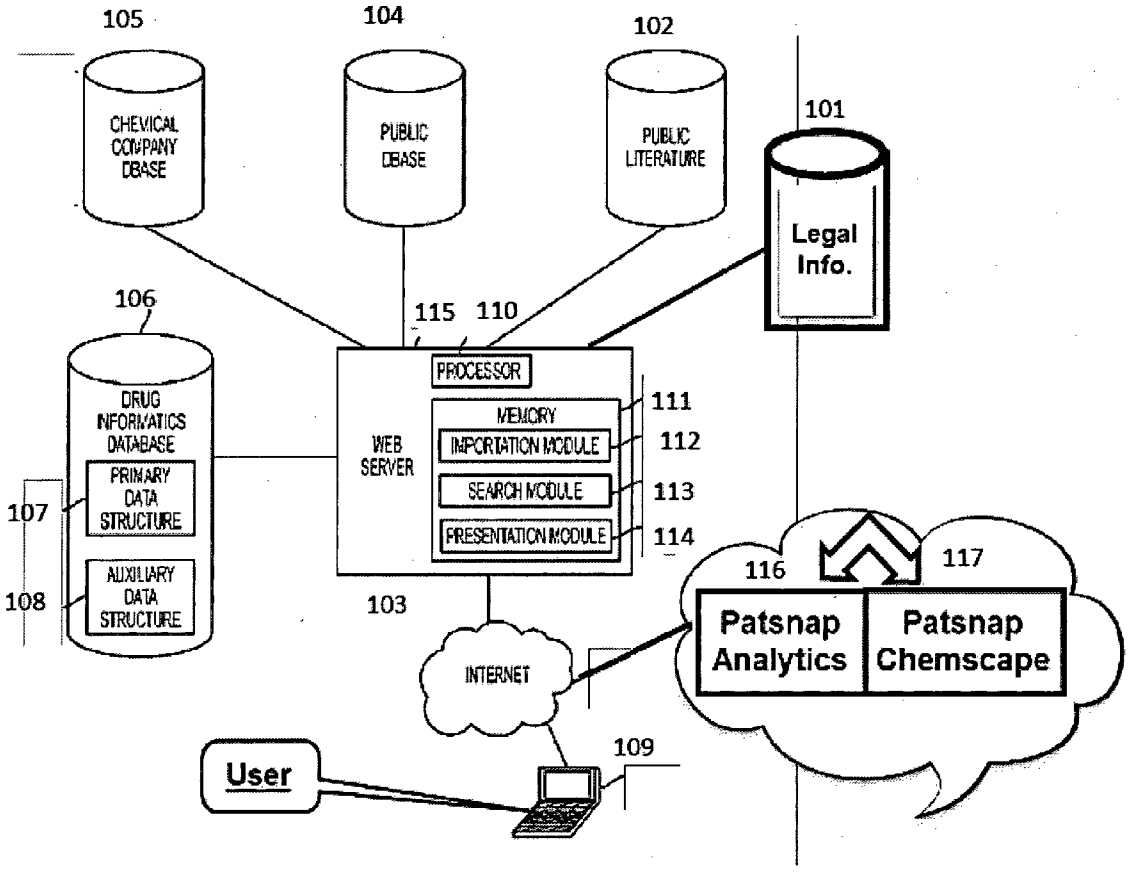
h) Accessing the secondary non-chemical data set records linked to the chemical records of the 2D-map via the 3D-map by clicking on one or several select graphic element via an inputting or a pointing device.

2. A method of automatically computing, mapping and accessing chemical structure similarities according to claim 1 further including the step of displaying the secondary data set records according to a particular and selectable task without exiting the search engine to access and visualize the secondary data set records.

3. A method of automatically computing, mapping and accessing chemical structure similarities according to claim 1 further including repeating step (c) by changing the method to evaluate a molecular similarity/dissimilarity.

4. A method of automatically computing, mapping and accessing chemical structure similarities where the 3D map is used to open and visualize simultaneously the chemical info and at least partially the non-chemical data including.

5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AUXILIARY DATA STRUCTURE
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108
115
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PROCESSOR
MEMORY
IMPORTATION MODULE
SEARCH MODULE
PRESENTATION MODULE
WEB SERVER
111
112
113
114
103
INTERNET
116
117
Patsnap Analytics
Patsnap Chemscape
User
109

Fig. 1

(19) **United States**
(12) **Reissued Patent**
Rosenblum et al.

(10) **Patent Number: US RE42,461 E**
(45) **Date of Reissued Patent: Jun. 14, 2011**

(54) **HYDROXY-SUBSTITUTED AZETIDINONE COMPOUNDS USEFUL AS HYPOCHOLESTEROLEMIC AGENTS**

(75) Inventors: **Stuart B. Rosenblum**, West Orange, NJ (US); **Sundeep Dugar**, San Jose, CA (US); **Duane A. Burnett**, Bernardsville, NJ (US); **John W. Clader**, Milton, VT (US); **Brian A. McKittrick**, New Vernon, NJ (US)

(73) Assignee: **Schering Corporation**, Kenilworth, NJ (US)

(21) Appl. No.: **12/797,341**

(22) PCT Filed: **Sep. 14, 1994**

(86) PCT No.: **PCT/US94/10099**

§ 371 (c)(1),
(2), (4) Date: **Mar. 18, 1996**

(87) PCT Pub. No.: **WO95/08532**

PCT Pub. Date: **Mar. 30, 1995**

Related U.S. Patent Documents

Reissue of:
(64) Patent No.: **Re. 37,721**
Issued: **May 28, 2002**
Appl. No.: **09/594,996**
Filed: **Jun. 15, 2000**

Which is a Reissue of:
(64) Patent No.: **5,767,115**
Issued: **Jun. 16, 1998**
Appl. No.: **08/617,751**
Filed: **Mar. 18, 1996**

(51) **Int. Cl.**
C07D 205/08 (2006.01)
A61P 9/10 (2006.01)

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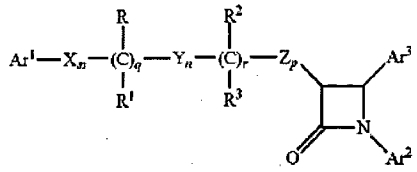
Allain et al., Enzymatic Determination of Total Serum Cholesterol, Clinical Chemical 20:470-475 (1974).

(Continued)

Primary Examiner — Mark L Berch
(74) *Attorney, Agent, or Firm* — Ropes & Gray LLP; James F. Haley, Jr.; Carl A. Morales

(57) **ABSTRACT**

Hydroxy-substituted azetidinone hypocholesterolemic agents of the formula



or a pharmaceutically acceptable salt thereof, wherein:
Ar^1 and Ar^2 are aryl or R^4-substituted aryl;
Ar^3 is aryl or R^5-substituted aryl;
X, Y and Z are —CH_2—, —CH(lower alkyl)— or —C(dilower alkyl)—;
R and R^2 are —OR^6, —O(CO)R^6, —O(CO)OR^9 or —O(CO)

Fig. 2

UNITED STATES DISTRICT COURT
FOR THE DISTRICT OF NEW JERSEY

SCHERING CORPORATION and, MSP SINGAPORE COMPANY LLC, *Plaintiffs/Counterclaim Defendants*, v. MYLAN PHARMACEUTICALS INC. *Defendant/Counterclaim Plaintiff.*	Civil Action No. 09-6383 (JLL)(MF) Civil Action No. 10-3085 (JLL)(MF)
SCHERING CORPORATION and MSP SINGAPORE COMPANY LLC, *Plaintiffs*, v. TEVA PHARMACEUTICALS USA, INC., *Defendant.*	Civil Action No. 10-1058 (JLL)(MF) Civil Action No. 10-4473 (JLL)(MF) (CONSOLIDATED)

FIRST AMENDED COMPLAINT

Plaintiffs Schering Corporation and MSP Singapore Company, LLC (collectively, "Plaintiffs"), by their attorneys, hereby amend their Complaint in *Schering Corporation and MSP Singapore Company LLC v. Mylan Pharmaceuticals Inc.*, Civ. A. No. 10-3085 (JLL)(MF) (D.I. 1), and allege as follows:

NATURE OF THE ACTION

1. This is an action for patent infringement under the patent laws of the United States, Title 35, United States Code, that arises out of the filing by Defendant Mylan Pharmaceuticals Inc. of Abbreviated New Drug Application ("ANDA") No. 201-790 with the U.S. Food and Drug Administration ("FDA") seeking approval to manufacture and sell a generic version of Zetia® prior to the expiration of U.S. Patent No. RE42,461 (the " '461 Patent") and U.S. Patent No. 5,846,966 (the ' '966 Patent). The '461 Patent recently issued on June 14, 2011 and is a reissue of U.S. Patent No. RE 37,721 (the " '721 Patent).

Fig. 3

DEPARTMENT OF HEALTH & HUMAN SERVICES

Food and Drug Administration
Silver Spring, MD 20993

ANDA 078560

APPROVAL

Glenmark Pharmaceuticals, Inc., USA
U.S. Agent for: Glenmark Pharmaceuticals Limited
750 Corporate Drive
Mahwah, NJ 07430
Attention: Kalpana Vanam
Vice President, Head of Regulatory Affairs, North America

Dear Sir or Madam:

This is in reference to your abbreviated new drug application (ANDA) dated October 25, 2007, submitted pursuant to section 505(j) of the Federal Food, Drug, and Cosmetic Act (the FD&C Act), for Ezetimibe Tablets, 10 mg.

We have completed the review of this ANDA and have concluded that adequate information has been presented to demonstrate that the drug is safe and effective for use as recommended in the submitted labeling. Accordingly the **ANDA is approved**, effective on the date of this letter. The Division of Bioequivalence has determined your Ezetimibe Tablets, 10 mg, to be bioequivalent and, therefore, therapeutically equivalent to the reference listed drug (RLD), Zetia (Ezetimibe), Tablets 10 mg, of MSD International GmbH (MSD). Your dissolution testing should be incorporated into the stability and quality control program using the same method proposed in your ANDA.

The RLD upon which you have based your ANDA, MSD's Zetia (Ezetimibe) Tablets, 10 mg, is subject to periods of patent protection. The following patents and expiration dates (with pediatric exclusivity added) are currently listed in the agency's publication titled Approved Drug Products with Therapeutic Equivalence Evaluations (the "Orange Book"):

U.S. Patent Number	Expiration Date
7,030,106 (the '106 patent)	July 25, 2022
7,612,058 (the '058 patent)	April 30, 2026
RE37,721 (the '721 patent)	April 25, 2017
RE42,461 (the '461 patent)	April 25, 2017

Fig. 4

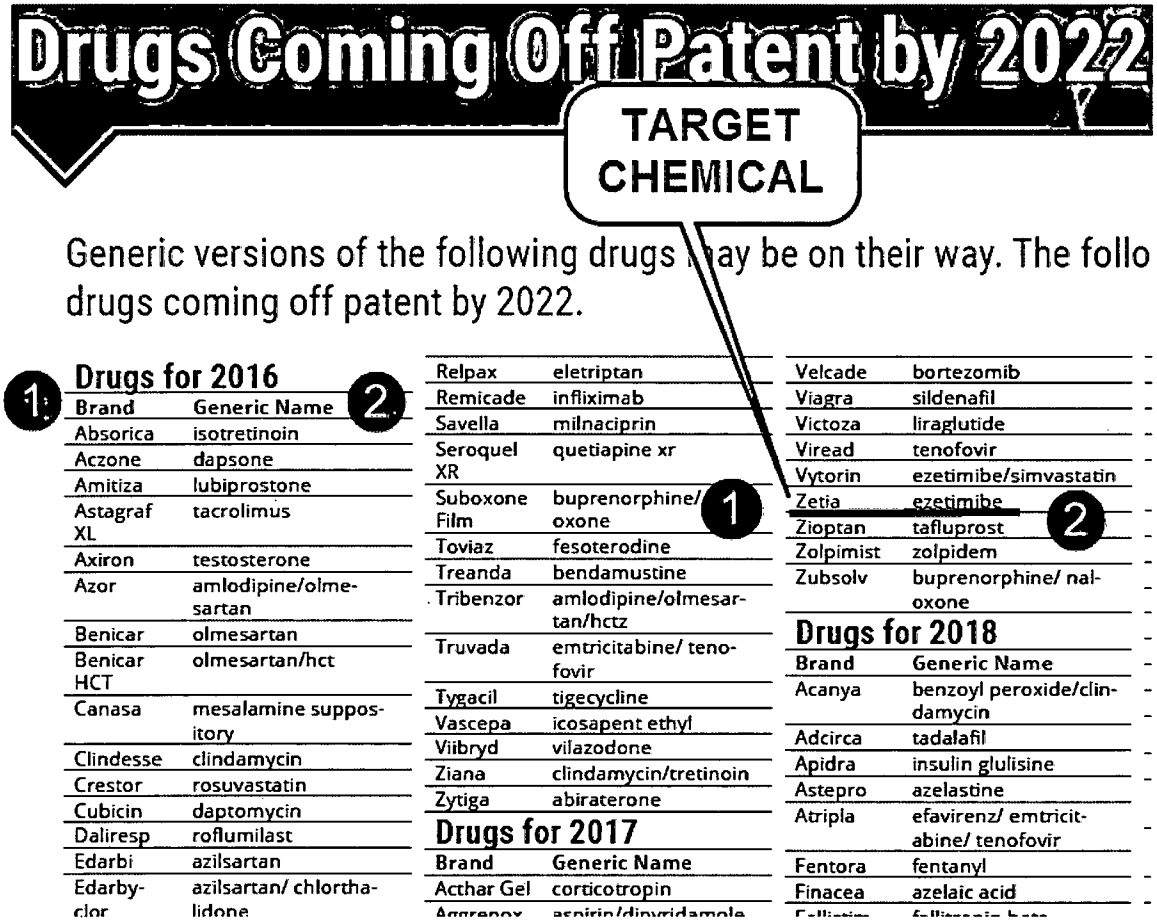


Fig. 5

	January 2008	February 2008
Cholesterol Management Market	20,363	18,947
Total Merck/Schering-Plough Franchise	3,194	2,773
VYTORIN	1,832	1,597
ZETIA	1,362	1,176

Source: IMS' *National Prescription Audit Plus (NPA+)*

Since the announcement of top-line results of the ENHANCE trial, IMS prescription data in the U.S. show that to date in 2008 prescriptions for VYTORIN and ZETIA have declined. Although the prescription data have shown some early signs of stabilization, there are limitations to this prescription data and it is too early to discern any trends from this data. It is likely that there will be fluctuations in IMS reported prescription volumes for VYTORIN and ZETIA before any trend can be identified. The Company believes that wholesalers, retail chains and other trade buyers are likely to respond to these fluctuations by changing their buying patterns or reducing their inventory levels.

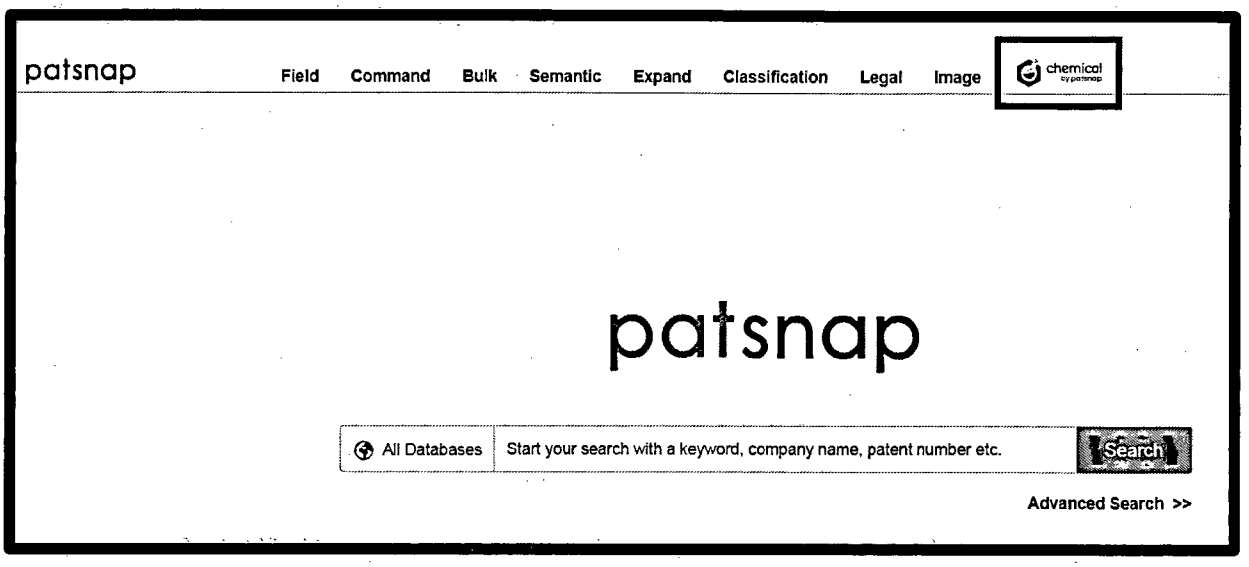
It is too early to determine the business and financial impact of these lower prescription volumes for 2008 or longer term. However, first quarter 2008 Merck/Schering-Plough cholesterol joint venture sales of VYTORIN and ZETIA in the U.S. will likely be negatively impacted. Schering-Plough accounts for the joint venture under the equity method.

Has pediatric exclusivity been granted for ZETIA and VYTORIN?

Yes, in February the Food & Drug Administration granted pediatric exclusivity for ZETIA and VYTORIN. The pediatric exclusivity will add 6-months of exclusivity to the patents, i.e., to April 25, 2017 for the composition of matter patent.

When do you expect the FDA to finish its review of sugammadex?

Fig.6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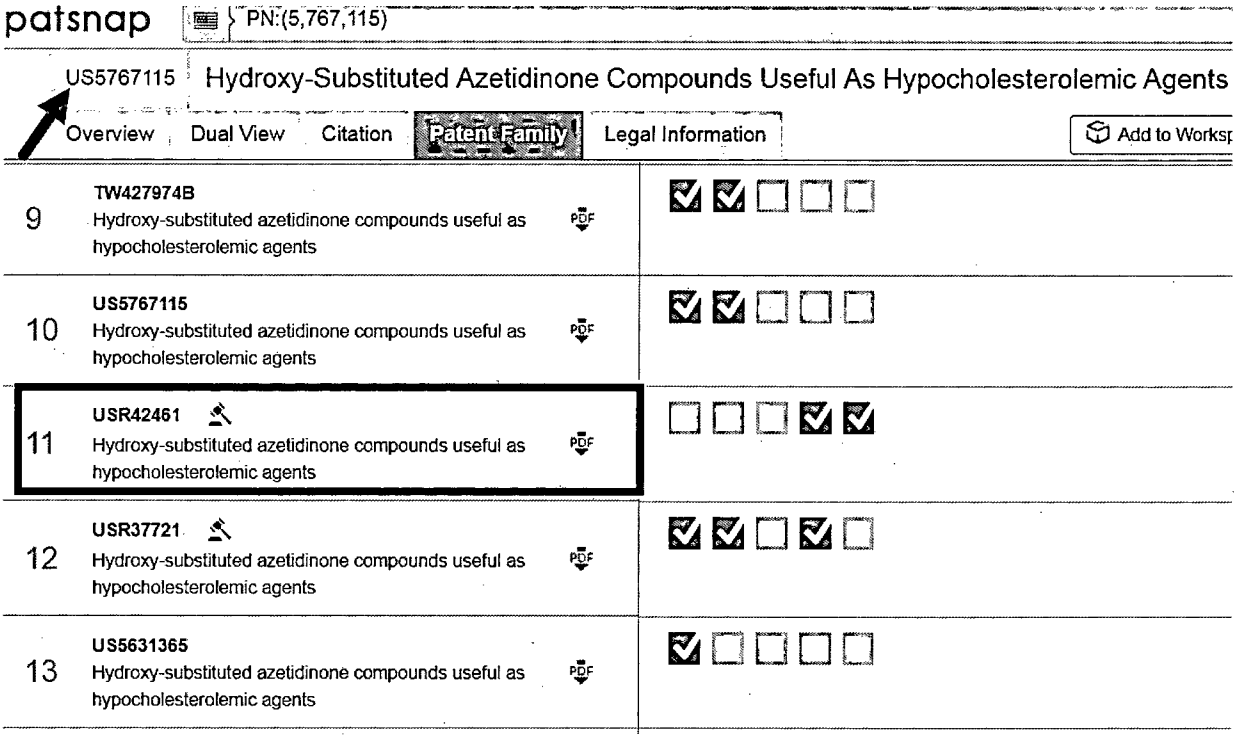
Advanced Search >>

Fig. 7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Overview
Dual View
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Patent Family
Legal Information
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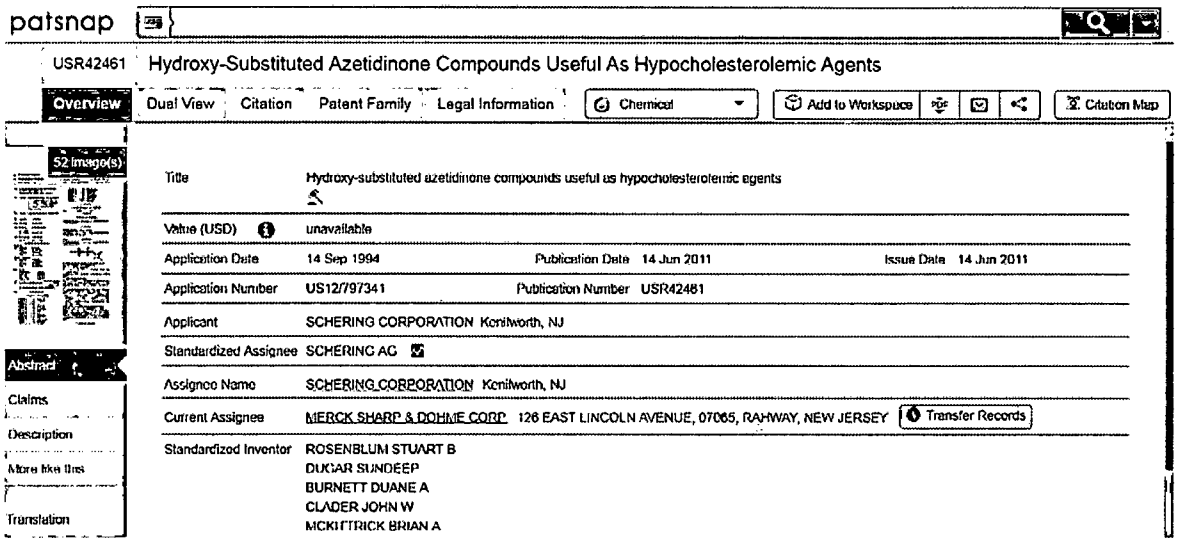
Hydroxy-substituted azetidinone compounds useful as hypocholesterolemic agents

Fig. 8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USR42461 Hydroxy-Substituted Azetidinone Compounds Useful As Hypocholesterolemic Agents
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Claims
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Application Date
14 Sep 1994
Publication Date
14 Jun 2011
Issue Date
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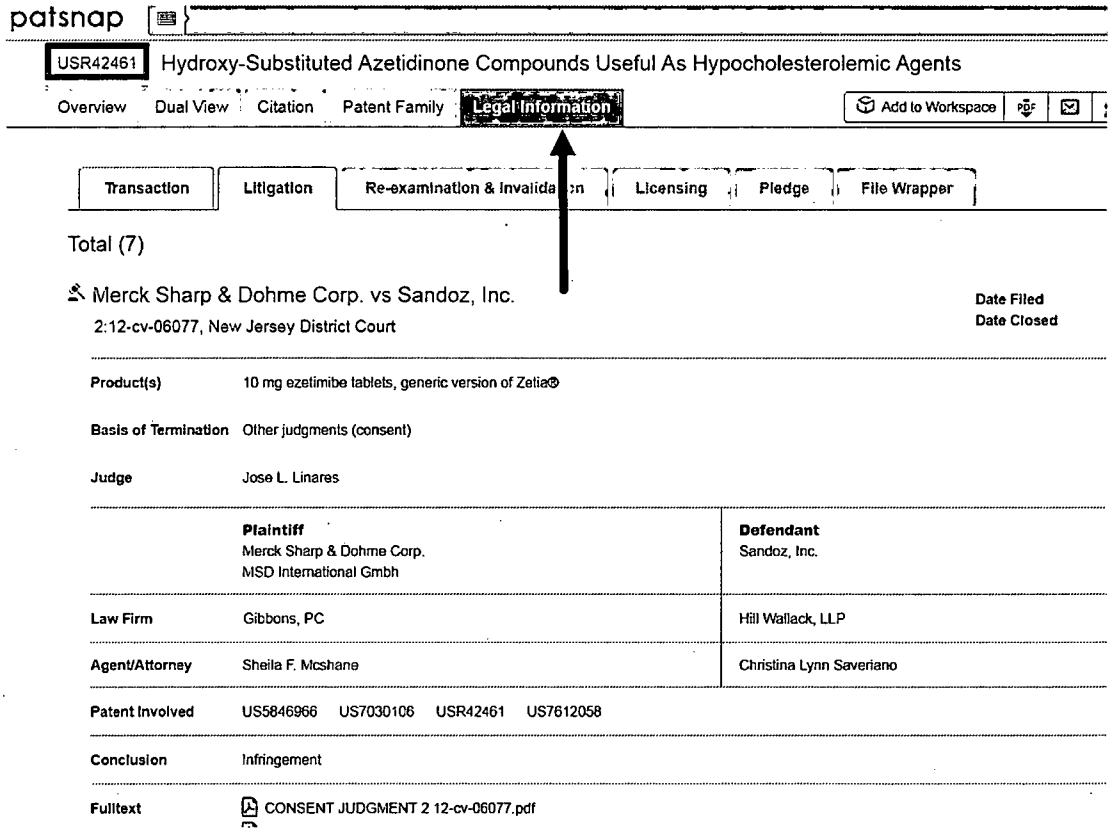
USR42461
Applicant
SCHERING CORPORATION Kenilworth, NJ
Standardized Assignee
SCHERING AG
Assignee Name
SCHERING CORPORATION Kenilworth, NJ
Current Assignee
MERCK SHARP & DOHME CORP 126 EAST LINCOLN AVENUE, 07065, RAHWAY, NEW JERSEY
Transfer Records
Standardized Inventor
ROSENBLUM STUART B
DUGAR SUNDEEP
BURNETT DUANE A
CLADER JOHN W
MCKITTRICK BRIAN A

Fig.9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Total (7)
Merck Sharp & Dohme Corp. vs Sandoz, Inc.
2:12-cv-06077, New Jersey District Court
Date Filed
Date Closed
Product(s)
10 mg ezetimibe tablets, generic version of Zetia®
Basis of Termination
Other judgments (consent)
Judge
Jose L. Linares
Plaintiff
Merck Sharp & Dohme Corp.
MSD International Gmbh
Defendant
Sandoz, Inc.
Law Firm
Gibbons, PC
Hill Wallack, LLP
Agent/Attorney
Sheila F. Mcshane
Christina Lynn Saveriano
Patent Involved
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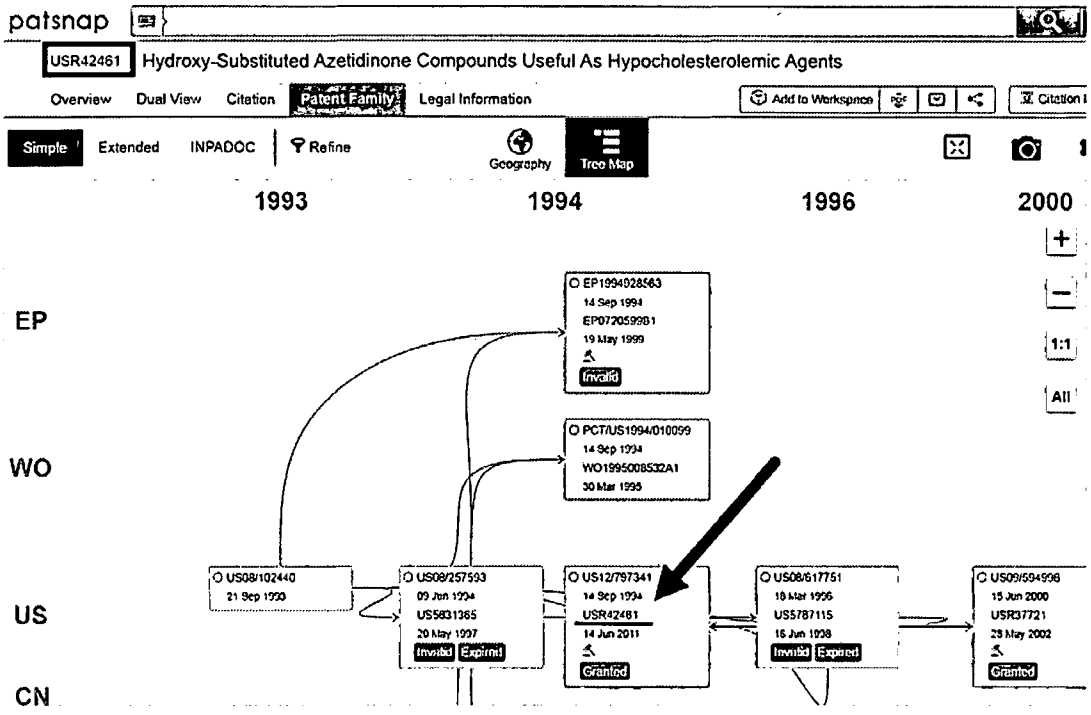
Conclusion
Infringement
Fulltext
CONSENT JUDGMENT 2 12-cv-06077.pdf

Fig. 10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15 Jun 2000
USR37721
28 May 2002
Granted

Fig. 11

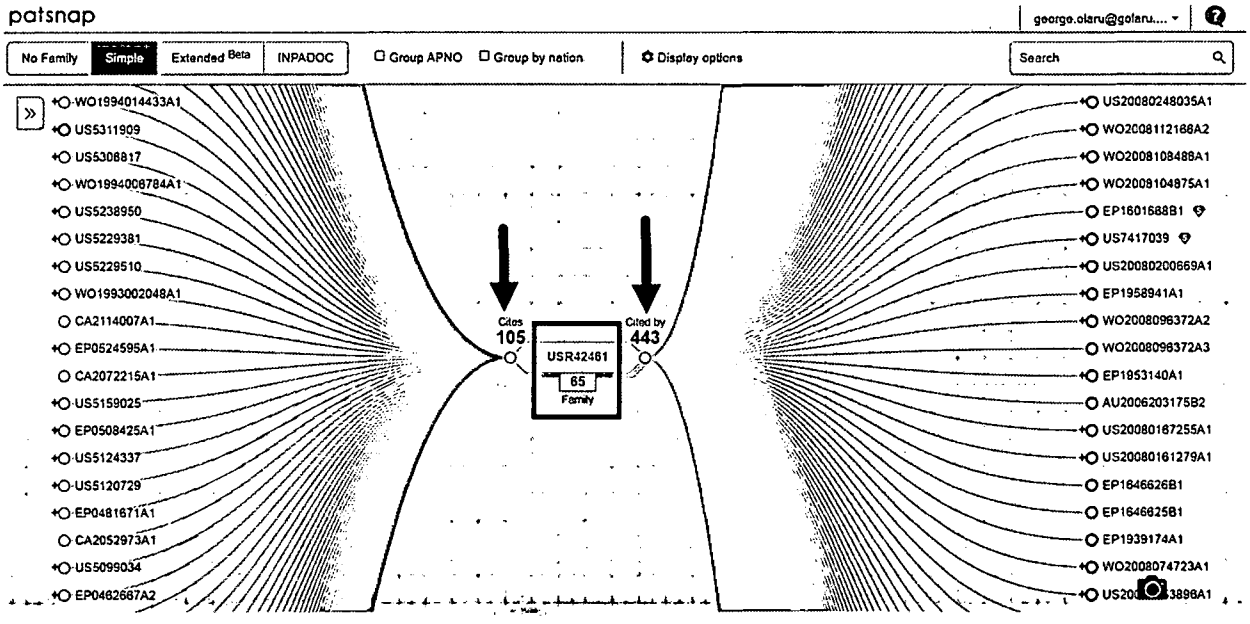
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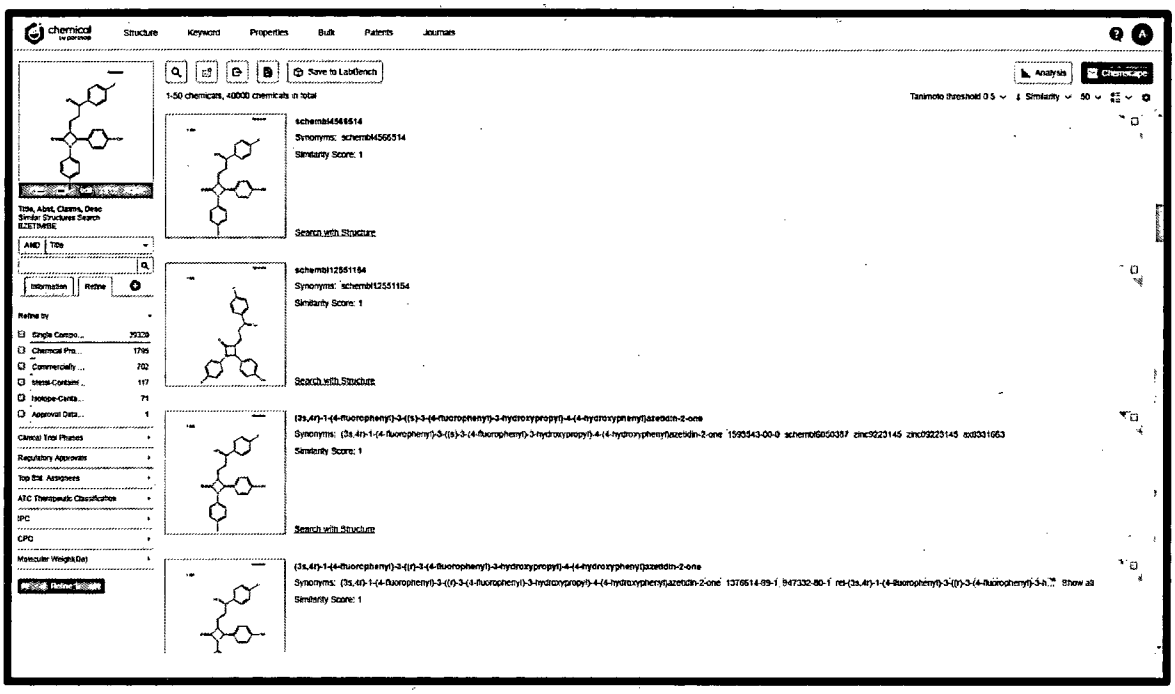
Fig. 12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Tanimoto threshold 0.5
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Synonyms: schembl4566514
Similarity Score: 1
Search with Structure
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Synonyms: schembl12551184
Similarity Score: 1
Search with Structure
Similarity Score: 1
Search with Structure
Similarity Score: 1
Title, Abst, Claims, Desc
Similar Structures Search
SUBSTRUCTURE
AND
Title
Information
Refine
Refine by
Single Compo...
Chemical Pro...
Commercially ...
Metal-Containi...
Isotope-Conta...
Approval Data...
Clinical Trial Phases
Regulatory Approvals
Top End Antiphoses
ATC Therapeutic Classification
IPC
CPC
Molecular Weight(Da)

Fig. 13

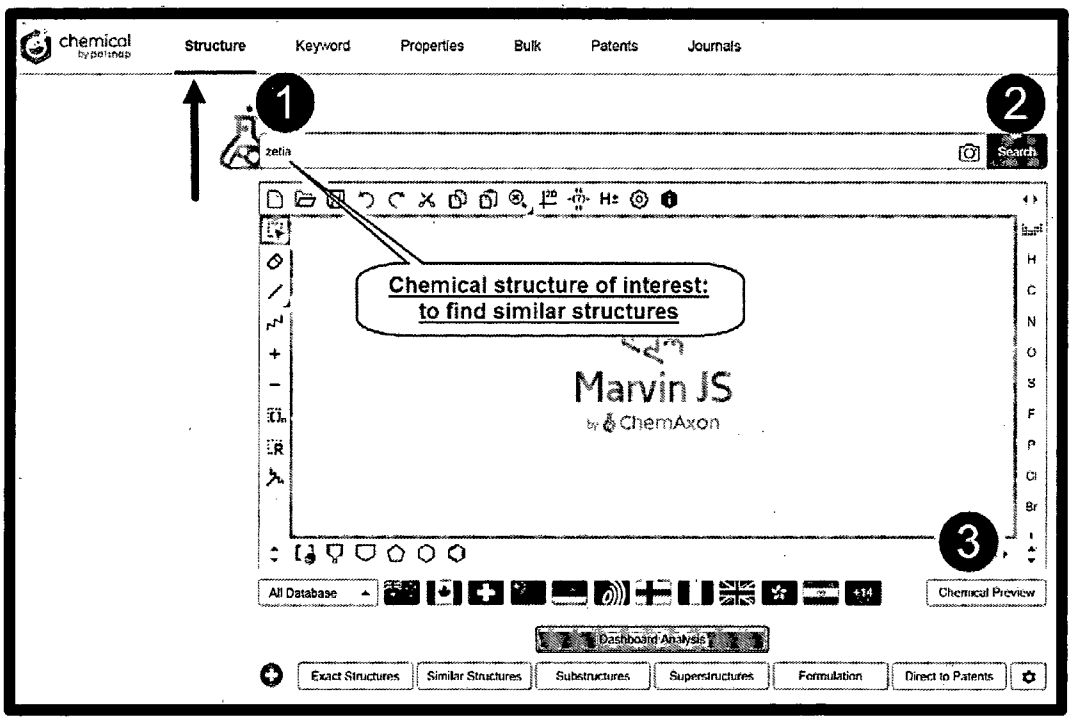
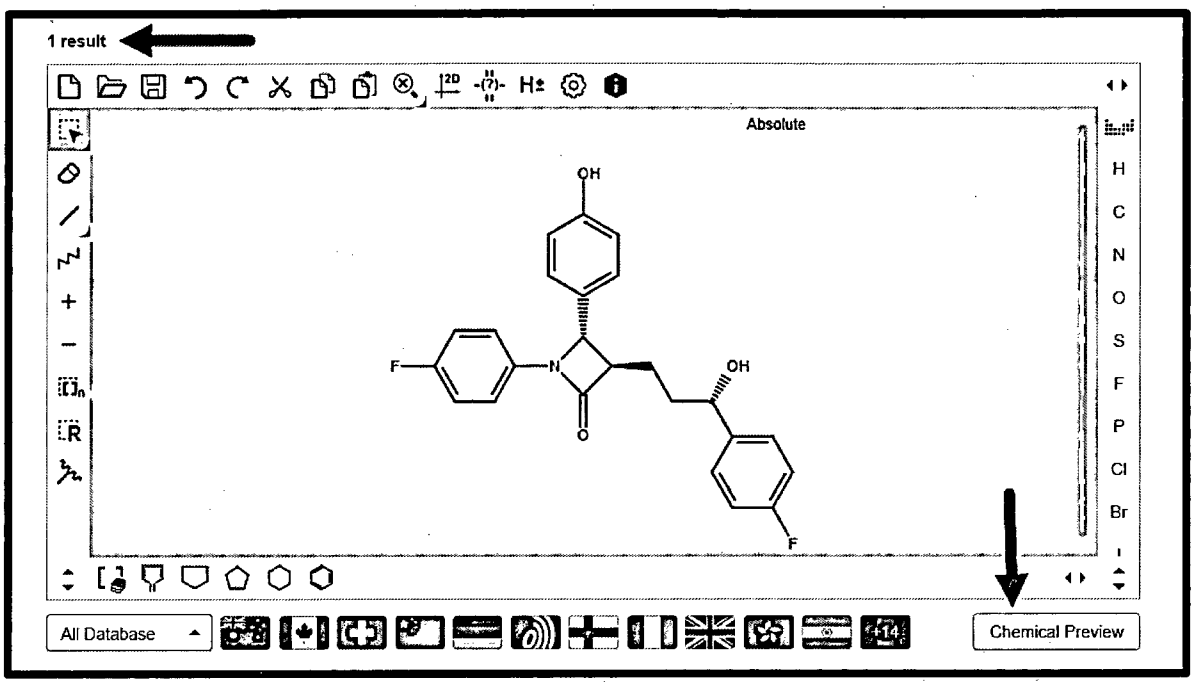

chemical
by peishep
Structure
Keyword
Properties
Bulk
Patents
Journals
1
2
zetia
Search
Chemical structure of interest:
to find similar structures
Marvin JS
by ChemAxon
3
All Database
Chemical Preview
Dashboard Analysis
Exact Structures
Similar Structures
Substructures
Superstructures
Formulation
Direct to Patents

Fig. 14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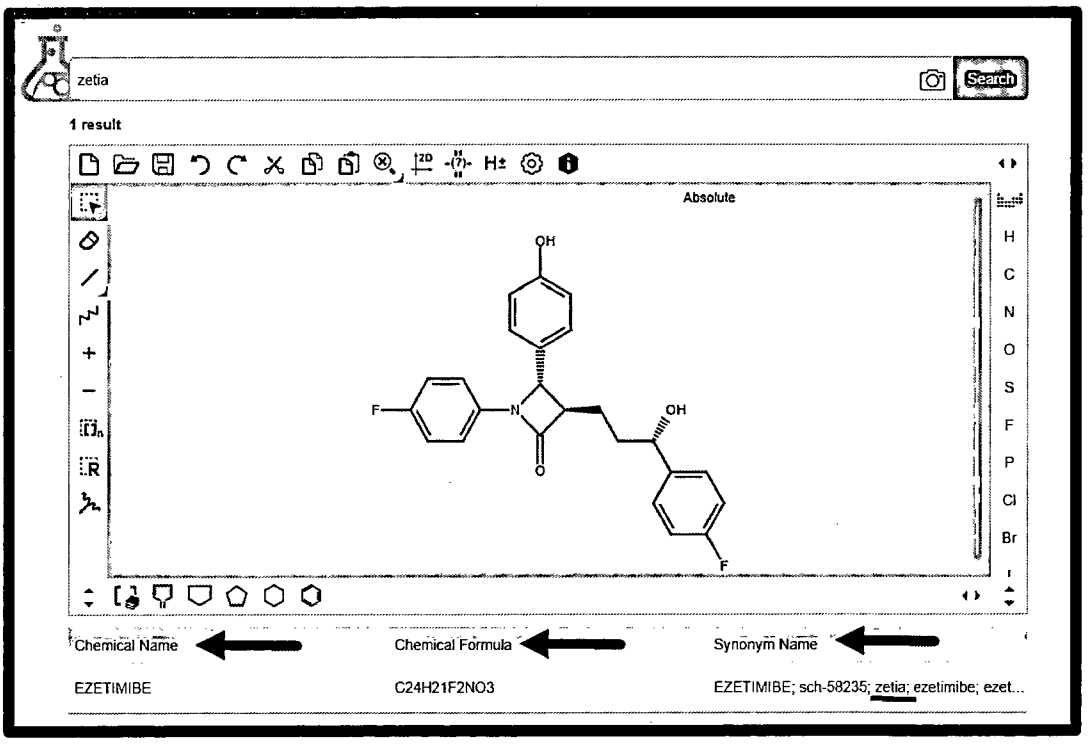
N
O
OH
F
H
C
N
O
S
F
P
Cl
Br
All Database
Chemical Preview

Fig. 15


zetia
Search
1 result
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H
C
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S
F
P
Cl
Br
Chemical Name
Chemical Formula
Synonym Name
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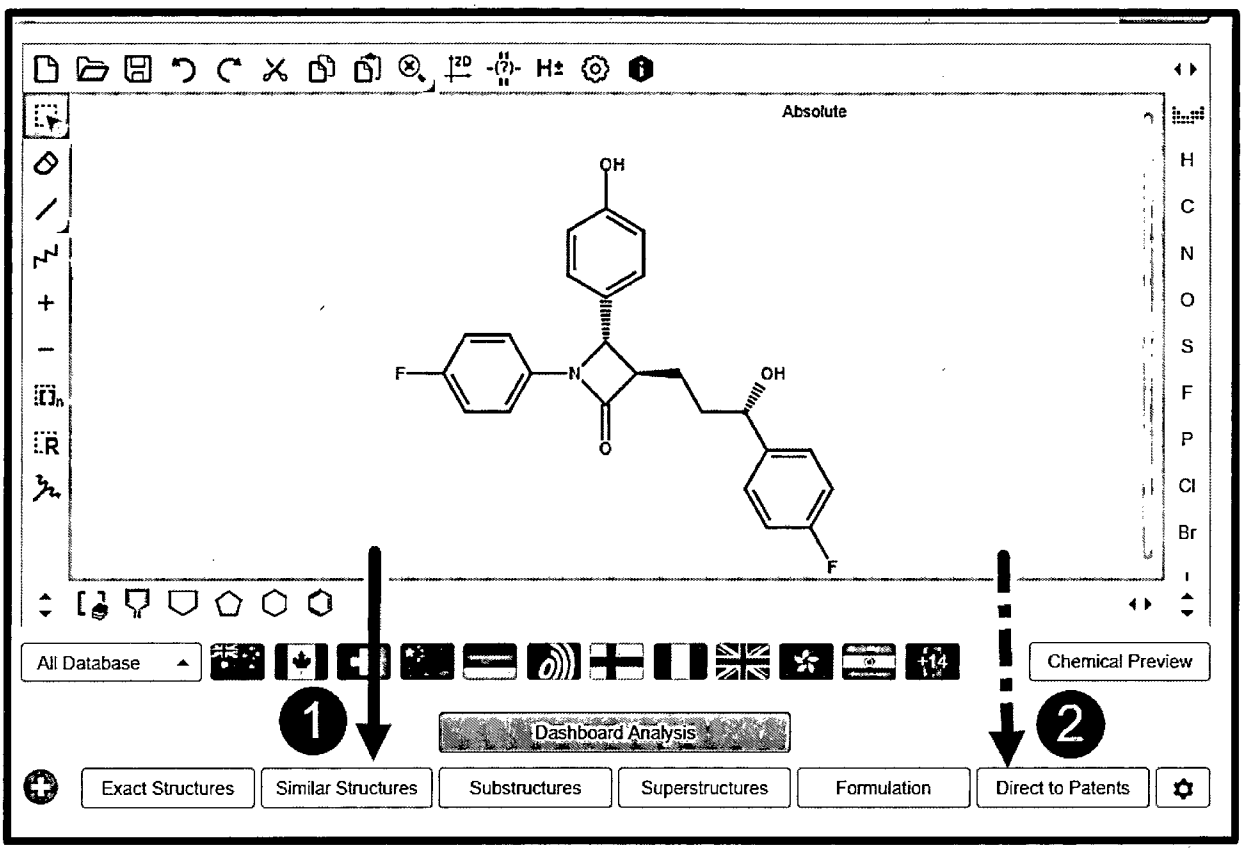
C24H21F2NO3
EZETIMIBE; sch-58235; zetia; ezetimibe; ezet...

Fig. 16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Cl
Br
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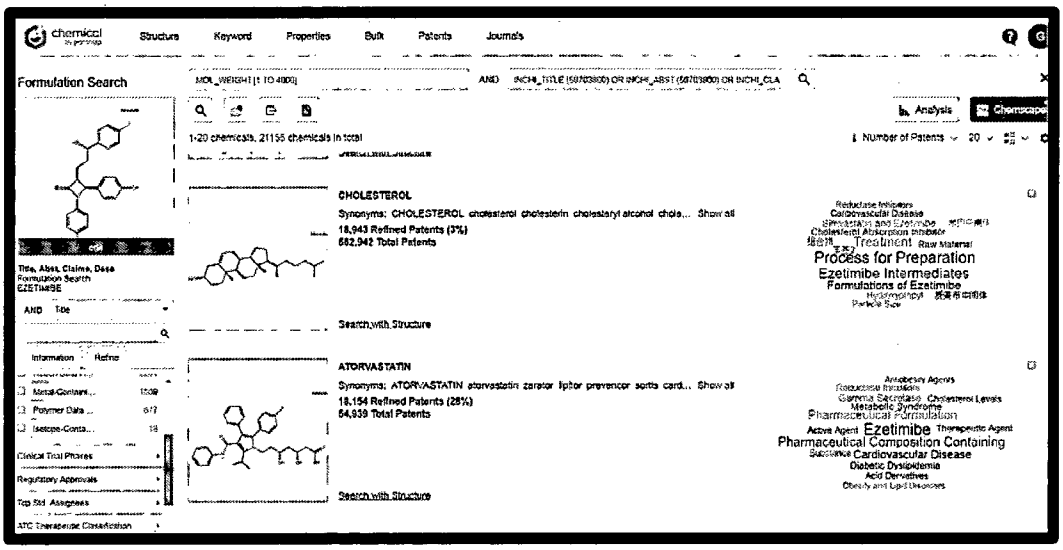
All Database
+14
Chemical Preview
1
Dashboard Analysis
2
Exact Structures
Similar Structures
Substructures
Superstructures
Formulation
Direct to Patents

Fig. 17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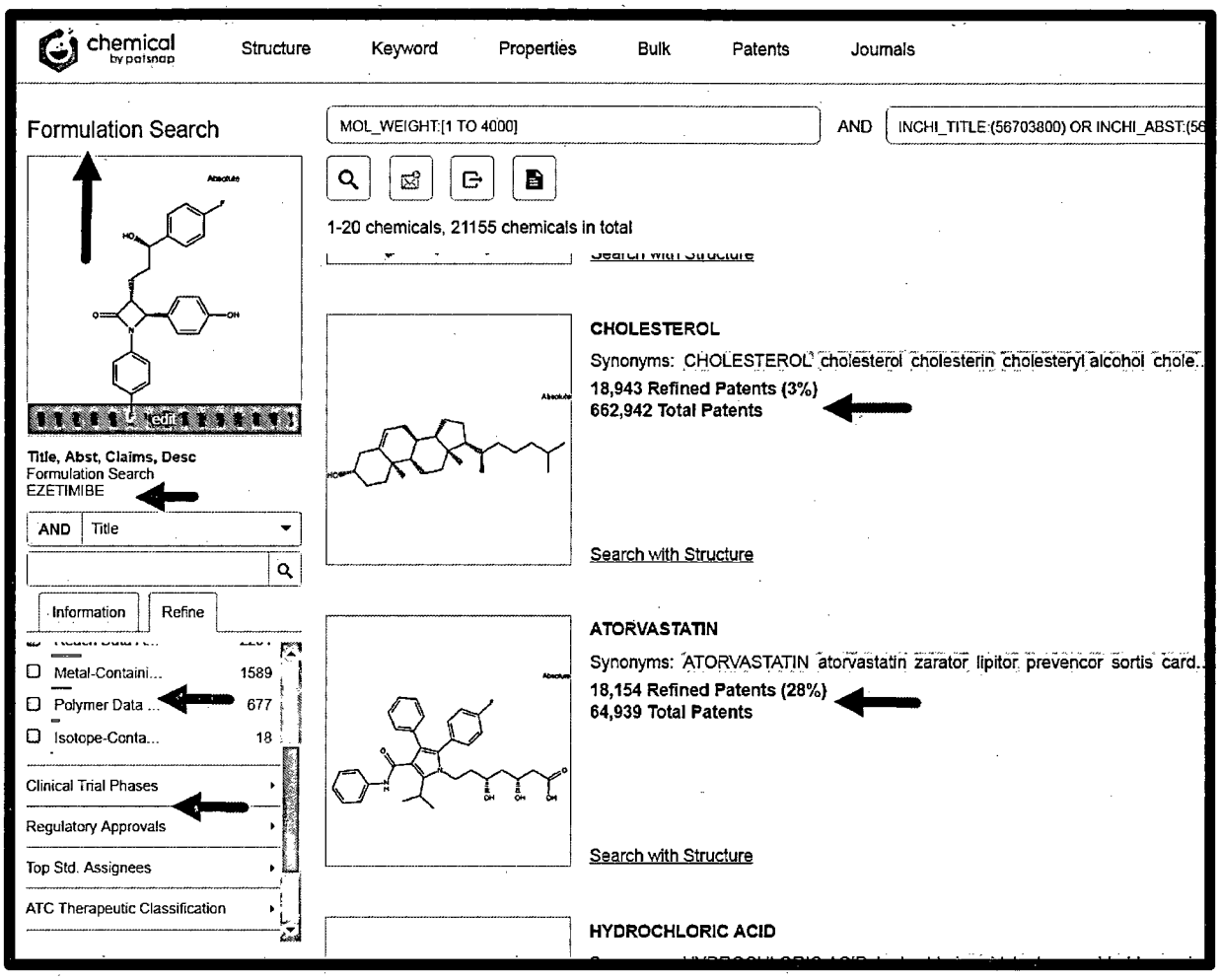
Keyword
Properties
Bulk
Patents
Journals
Formulation Search
CHOLESTEROL
ATORVASTATIN
Process for Preparation
Ezetimibe Intermediates
Formulations of Ezetimibe
Ezetimibe
Pharmaceutical Composition Containing

Fig. 18


chemical by patsnap
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Keyword
Properties
Bulk
Patents
Journals
Formulation Search
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AND
INCHI_TITLE:(56703800) OR INCHI_ABST:(56
1-20 chemicals, 21155 chemicals in total
CHOLESTEROL
Synonyms: CHOLESTEROL cholesterol cholesterin cholesteryl alcohol chole..
18,943 Refined Patents (3%)
662,942 Total Patents
Search with Structure
Title, Abst, Claims, Desc
Formulation Search
EZETIMIBE
AND
Title
Information
Refine
Metal-Containi... 1589
Polymer Data ... 677
Isotope-Conta... 18
Clinical Trial Phases
Regulatory Approvals
Top Std. Assignees
ATC Therapeutic Classification
ATORVASTATIN
Synonyms: ATORVASTATIN atorvastatin zarator lipitor prevencor sortis card..
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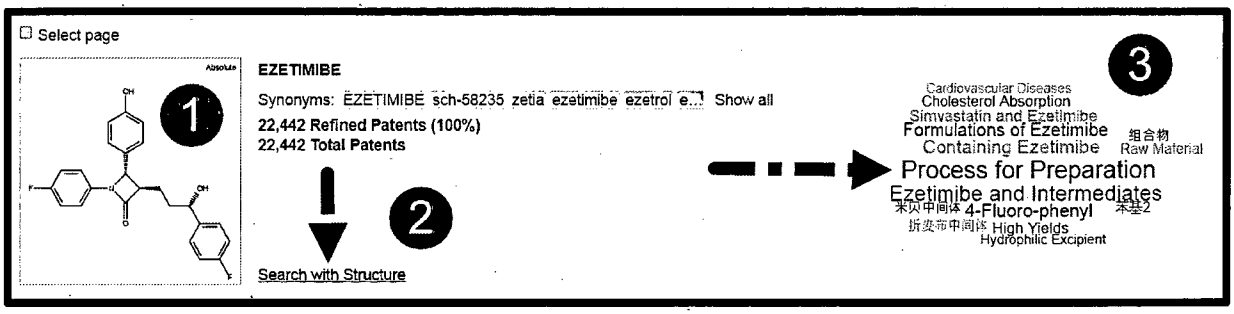
64,939 Total Patents
Search with Structure
HYDROCHLORIC ACID

Fig. 19


Select page
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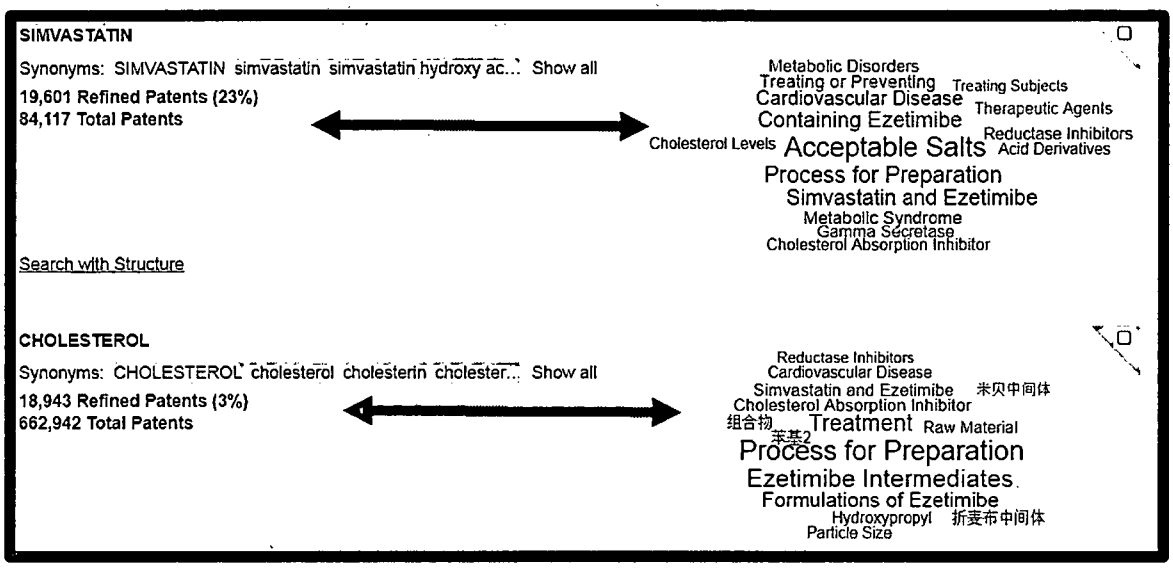
Synonyms: EZETIMIBE sch-58235 zetia ezetimibe ezetrol e..
Show all
22,442 Refined Patents (100%)
22,442 Total Patents
Search with Structure
1
2
3
Cardiovascular Diseases
Cholesterol Absorption
Simvastatin and Ezetimibe
Formulations of Ezetimibe
Containing Ezetimibe
Process for Preparation
Ezetimibe and Intermediates
4-Fluoro-phenyl
High Yields
Hydrophilic Excipient
Raw Material

Fig. 20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Synonyms: SIMVASTATIN simvastatin simvastatin hydroxy ac... Show all
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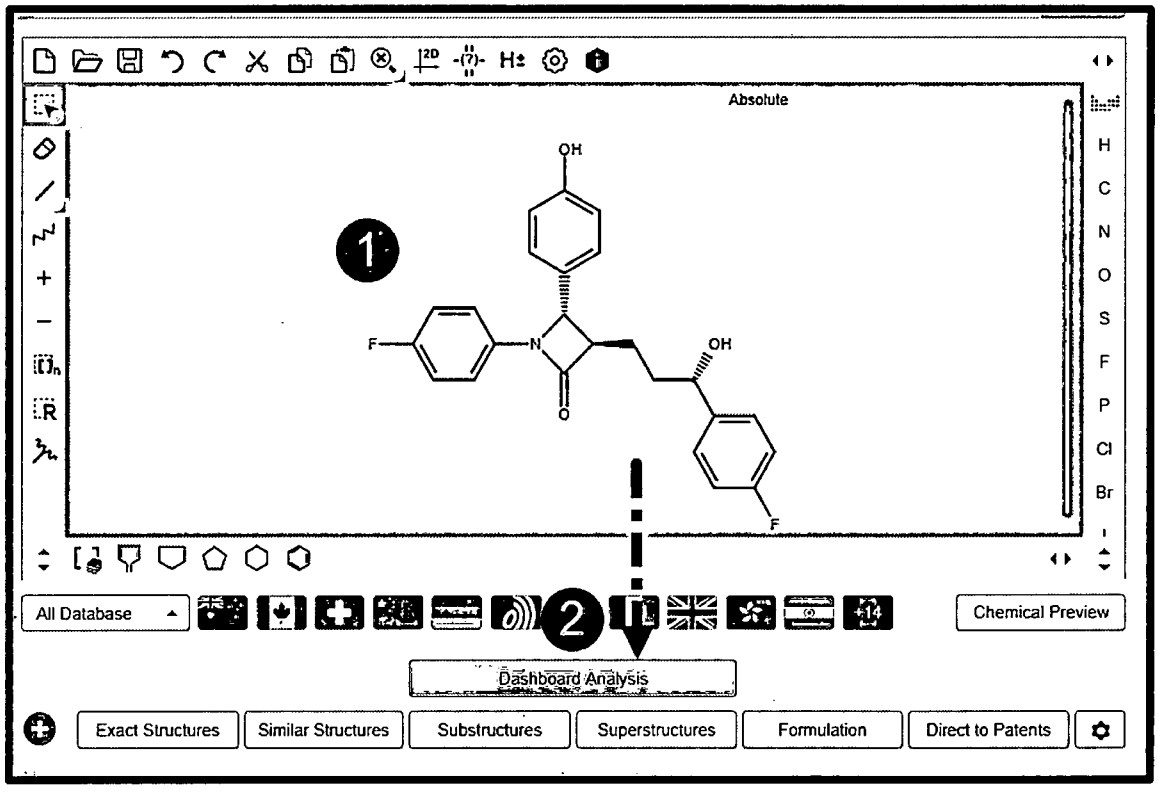
84,117 Total Patents
Search with Structure
Metabolic Disorders
Treating or Preventing
Treating Subjects
Cardiovascular Disease
Therapeutic Agents
Containing Ezetimibe
Reductase Inhibitors
Cholesterol Levels
Acceptable Salts
Acid Derivatives
Process for Preparation
Simvastatin and Ezetimibe
Metabolic Syndrome
Gamma Secretase
Cholesterol Absorption Inhibitor
CHOLESTEROL
Synonyms: CHOLESTEROL cholesterol cholesterin cholester... Show all
18,943 Refined Patents (3%)
662,942 Total Patents
Reductase Inhibitors
Cardiovascular Disease
Simvastatin and Ezetimibe
Cholesterol Absorption Inhibitor
Treatment
Raw Material
Process for Preparation
Ezetimibe Intermediates
Formulations of Ezetimibe
Hydroxypropyl
Particle Size

Fig. 21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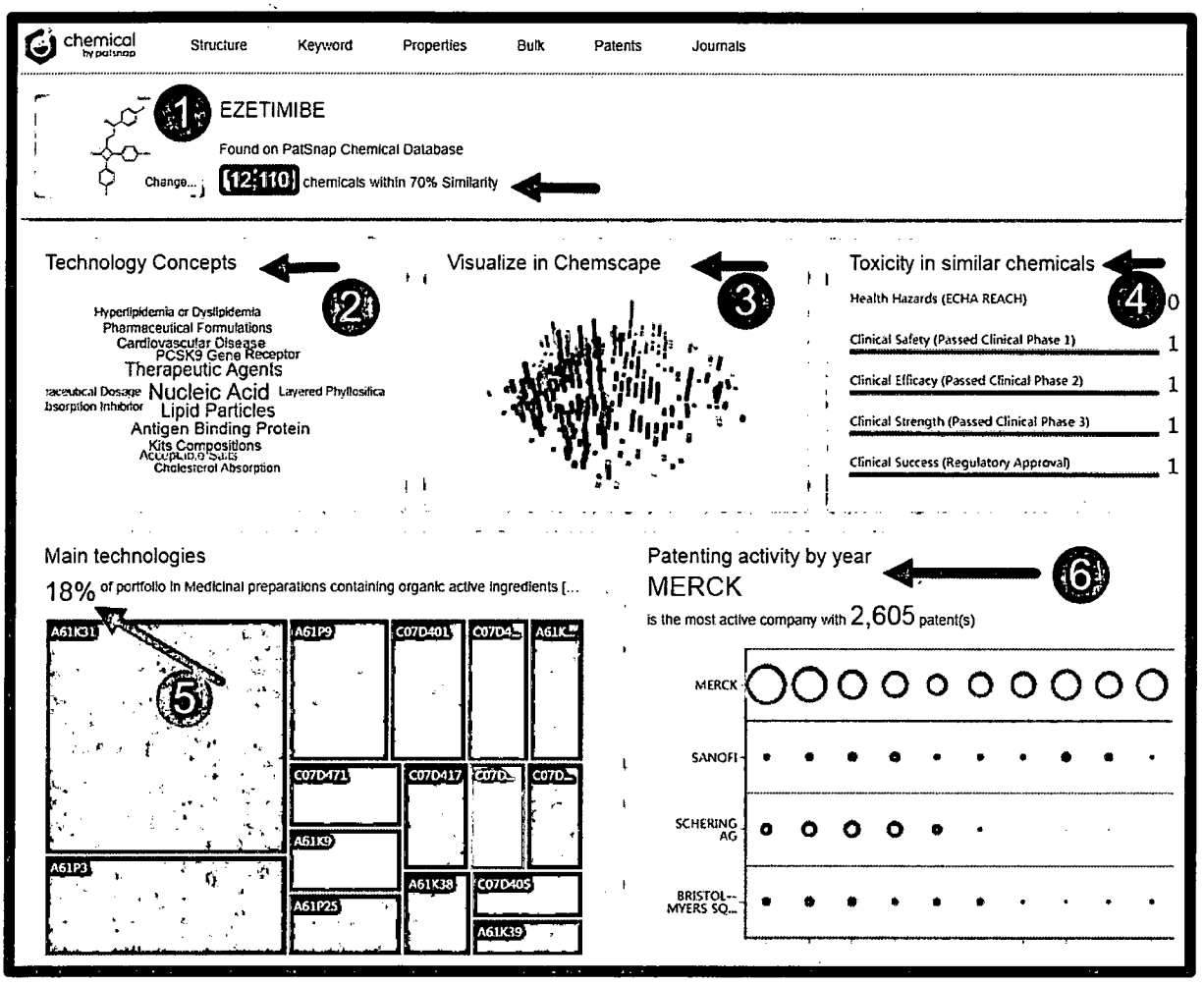
F
N
OH
O
F
1
2
All Database
Chemical Preview
Dashboard Analysis
Exact Structures
Similar Structures
Substructures
Superstructures
Formulation
Direct to Patents

Fig. 22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Structure
Keyword
Properties
Bulk
Patents
Journals
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Found on PatSnap Chemical Database
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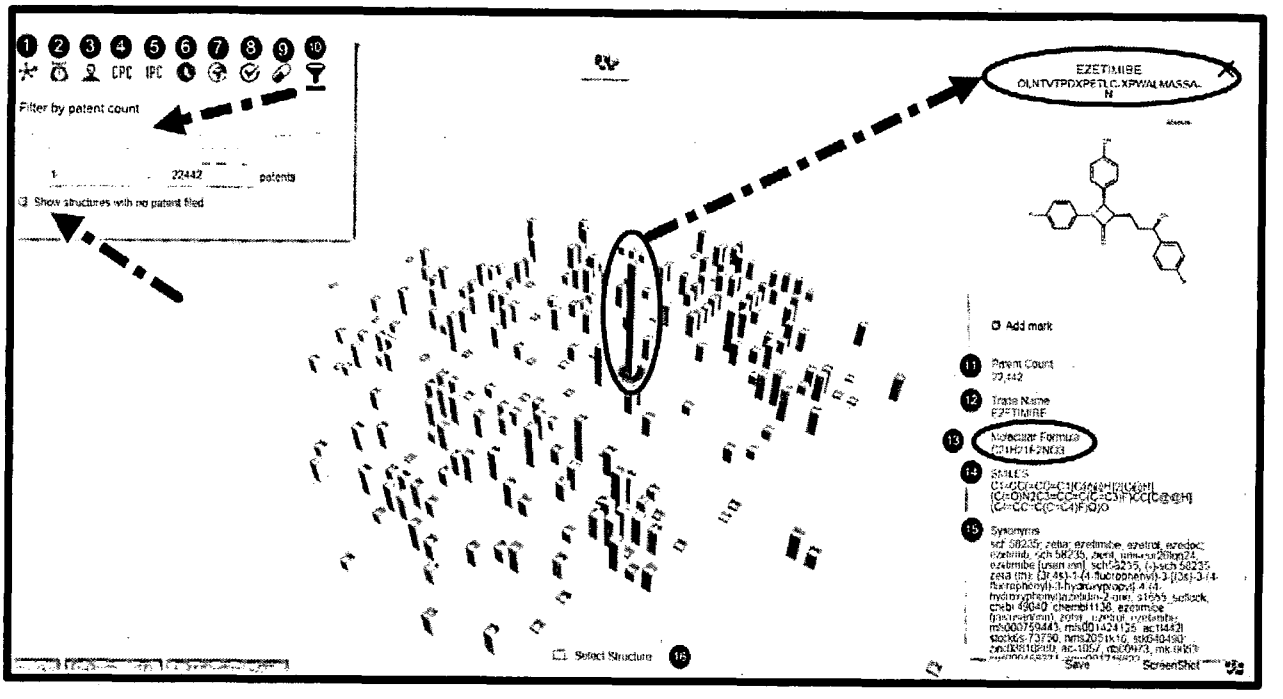
Technology Concepts
2
Hyperlipidemia or Dyslipidemia
Pharmaceutical Formulations
Cardiovascular Disease
PCSK9 Gene Receptor
Therapeutic Agents
Nucleic Acid
Lipid Particles
Antigen Binding Protein
Kits Compositions
Cholesterol Absorption
Visualize in Chemscape
3
Toxicity in similar chemicals
Health Hazards (ECHA REACH)
4
0
Clinical Safety (Passed Clinical Phase 1)
1
Clinical Efficacy (Passed Clinical Phase 2)
1
Clinical Strength (Passed Clinical Phase 3)
1
Clinical Success (Regulatory Approval)
1
Main technologies
18% of portfolio in Medicinal preparations containing organic active ingredients [...
5
A61K31
A61P9
C07D401
A61K9
A61P3
A61P25
A61K38
C07D405
A61K39
Patenting activity by year
6
MERCK
is the most active company with 2,605 patent(s)
MERCK
SANOFI
SCHERING AG
BRISTOL-- MYERS SQ...

Fig. 23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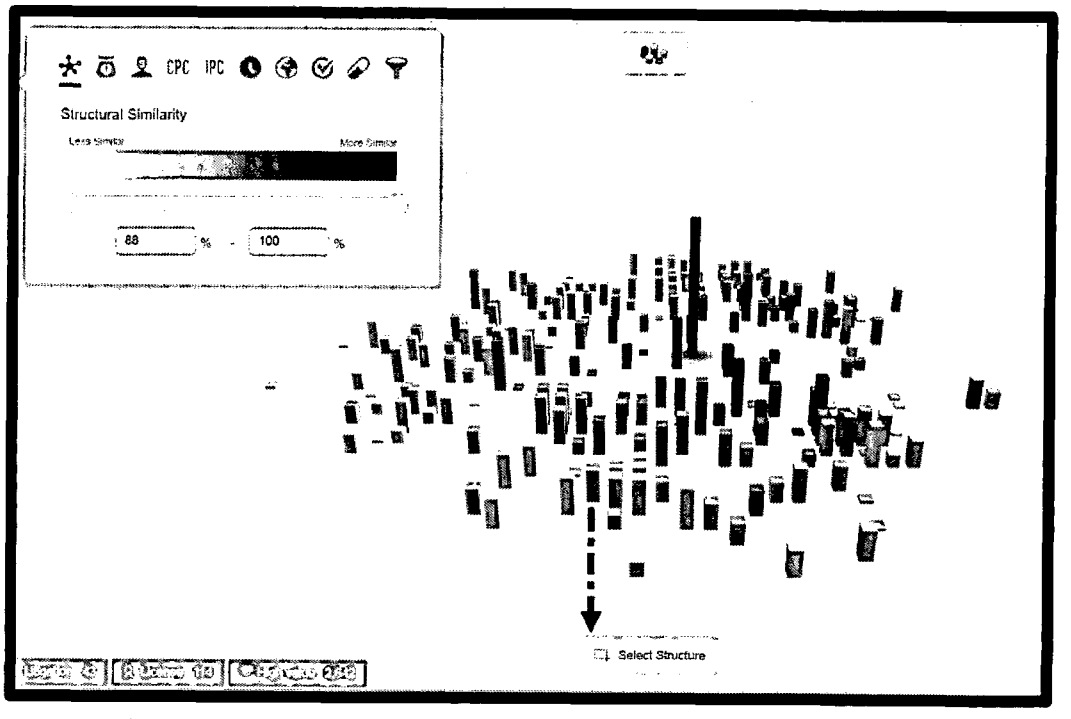
IPC
Filter by patent count
22442
patents
Show structures with no patent filed
EZETIMIBE
Add mark
Patent Count
Trade Name
EZETIMIBE
Molecular Formula
Select Structure
Save
ScreenShot

Fig. 24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IPC
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More Similar
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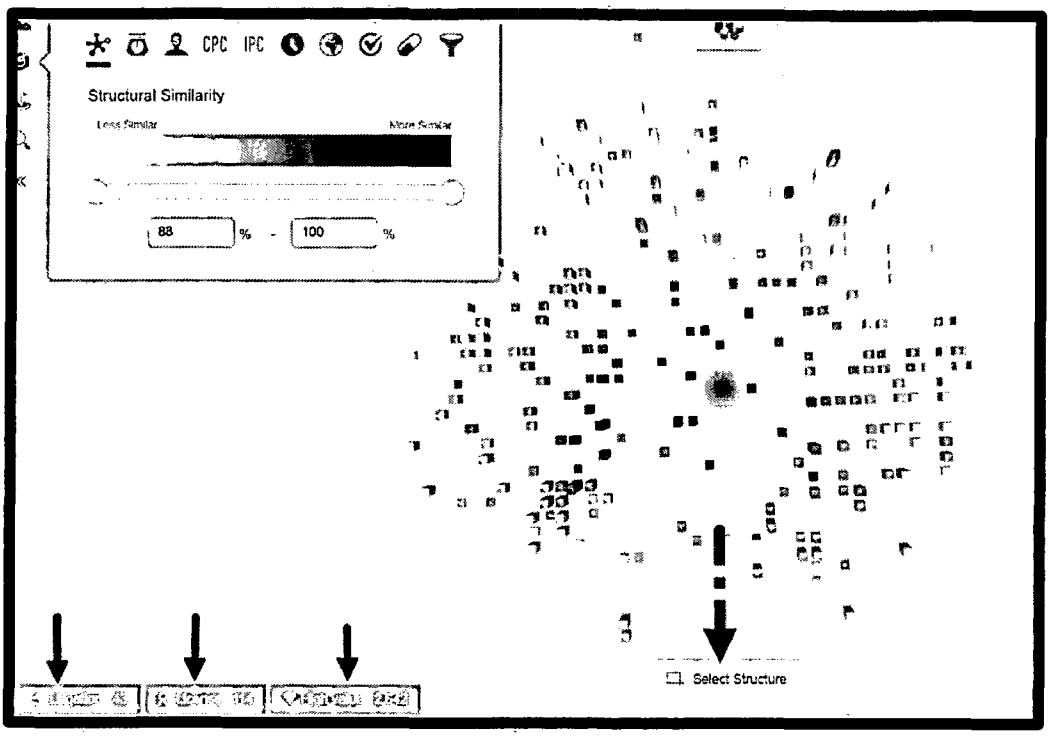
%
100
%
Select Structure

Fig. 25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IPC
Structural Similarity
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More Similar
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%
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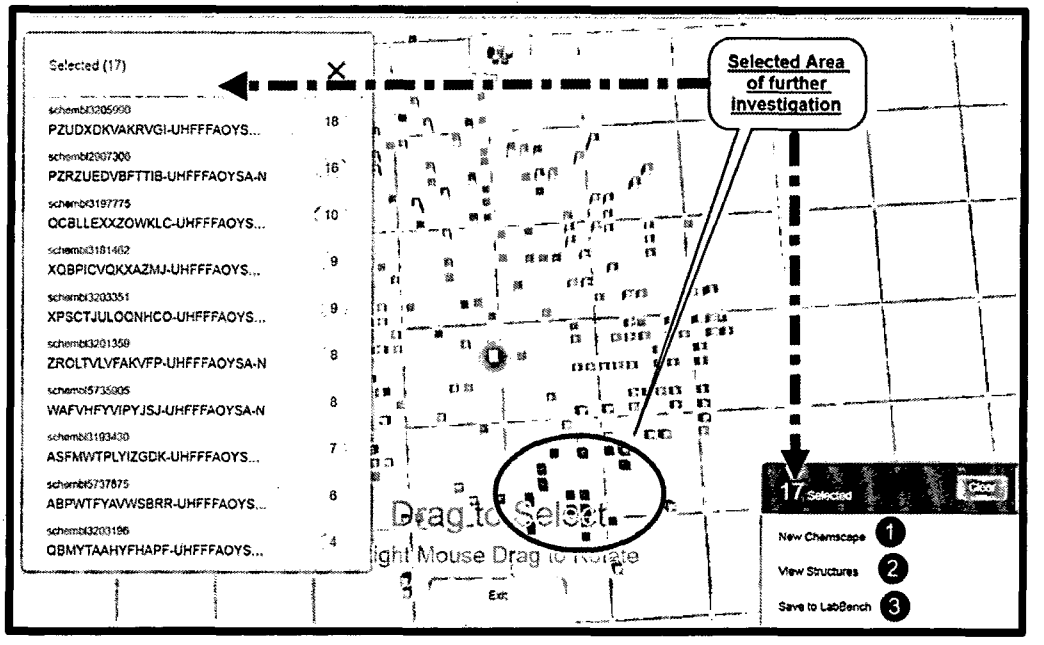
%
Select Structure

Fig. 26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QCBLLEXXZOWKLC-UHFFFAOYS...
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XQBPICVQKXAZMJ-UHFFFAOYS...
9
schembl3203351
XPSCTJULOCNHCO-UHFFFAOYS...
9
schembl3201359
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schembl5735905
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8
schembl3193430
ASFMWTPLYIZGDK-UHFFFAOYS...
7
schembl5737875
ABPWTFYAVWSBRR-UHFFFAOYS...
6
schembl3203196
QBMYTAAHYFHAPF-UHFFFAOYS...
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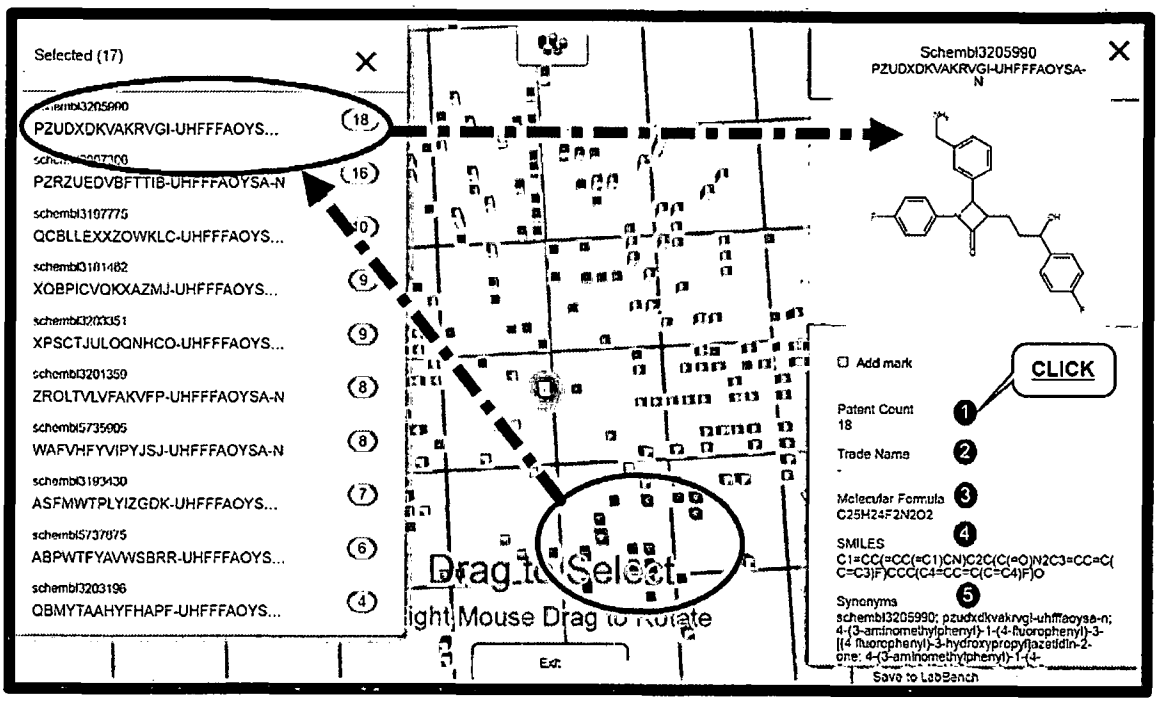
Selected Area of further investigation
Drag to Select
17 Selected
Clear
New Chemscape 1
View Structures 2
Save to LabBench 3

Fig. 27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QBMYTAAHYFHAPF-UHFFFAOYS...
Schembl3205990
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Trade Name
Molecular Formula
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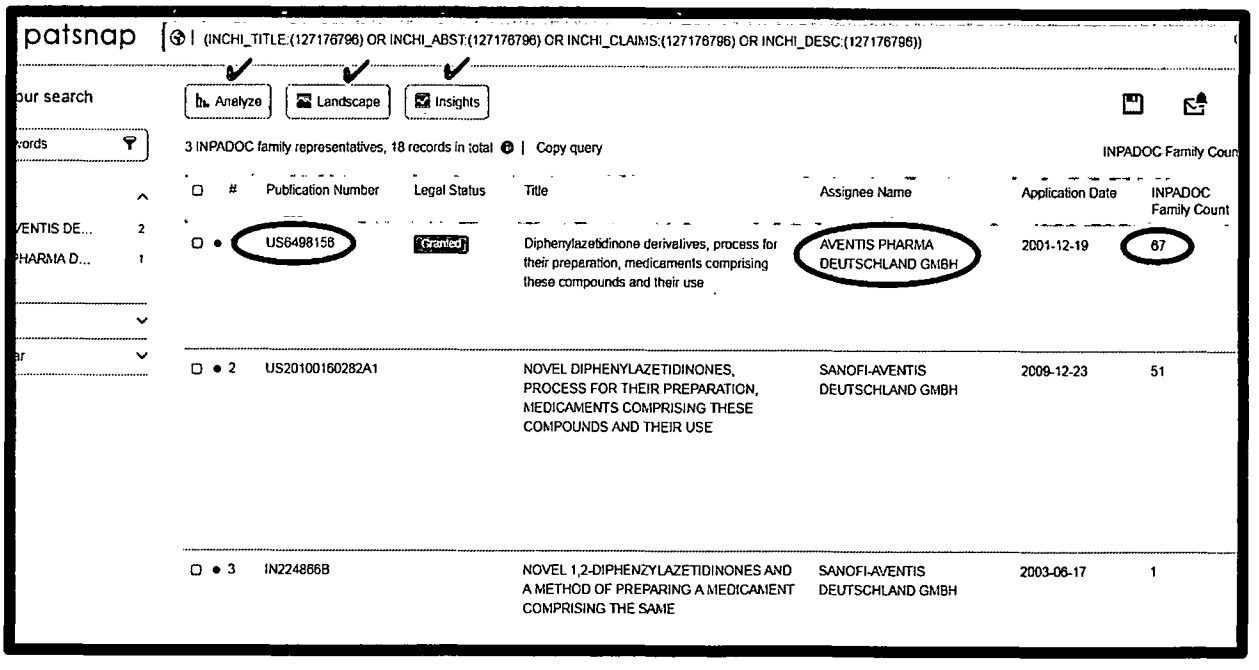
SMILES
Synonyms
Save to LabBench

Fig. 28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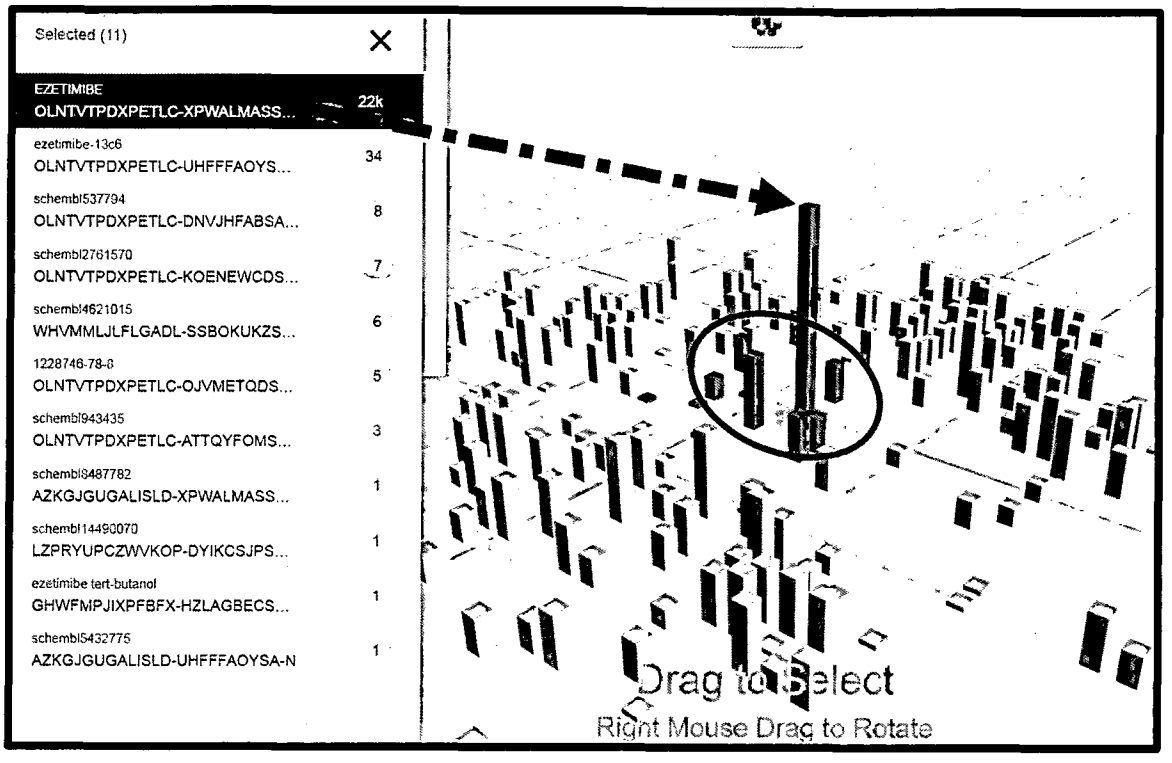
Analyze
Landscape
Insights
3 INPADOC family representatives, 18 records in total | Copy query
Publication Number Legal Status Title Assignee Name Application Date INPADOC Family Count
US6498158 Granted Diphenylazetidinone derivatives, process for their preparation, medicaments comprising these compounds and their use AVENTIS PHARMA DEUTSCHLAND GMBH 2001-12-19 67
2 US20100160282A1 NOVEL DIPHENYLAZETIDINONES, PROCESS FOR THEIR PREPARATION, MEDICAMENTS COMPRISING THESE COMPOUNDS AND THEIR USE SANOFI-AVENTIS DEUTSCHLAND GMBH 2009-12-23 51
3 IN224866B NOVEL 1,2-DIPHENZYLAZETIDINONES AND A METHOD OF PREPARING A MEDICAMENT COMPRISING THE SAME SANOFI-AVENTIS DEUTSCHLAND GMBH 2003-06-17 1

Fig. 29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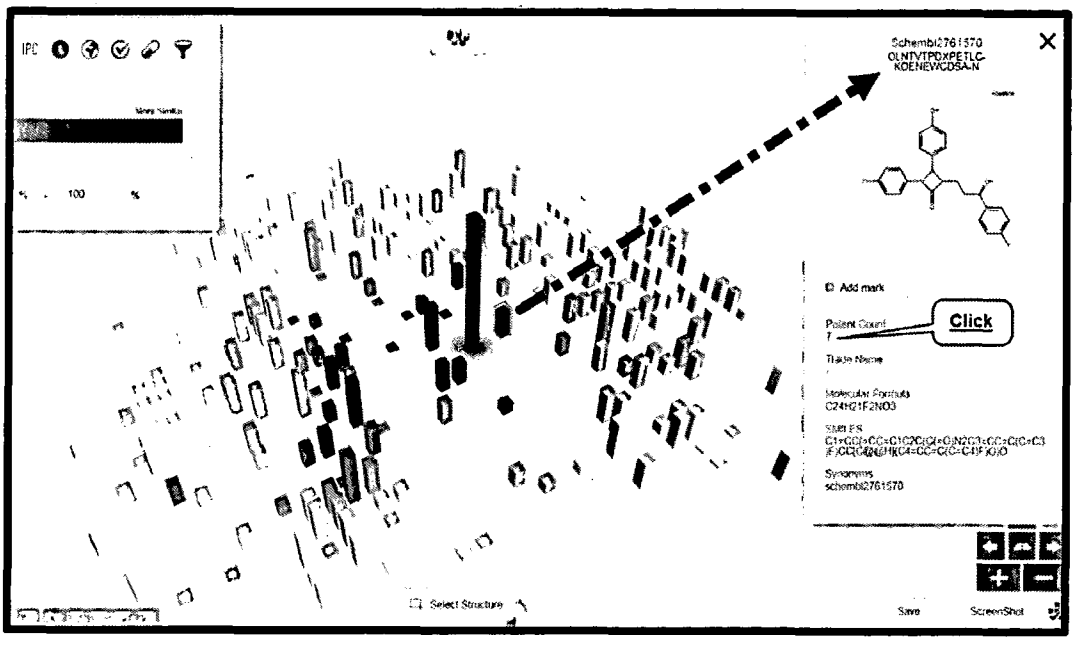
Right Mouse Drag to Rotate

Fig. 30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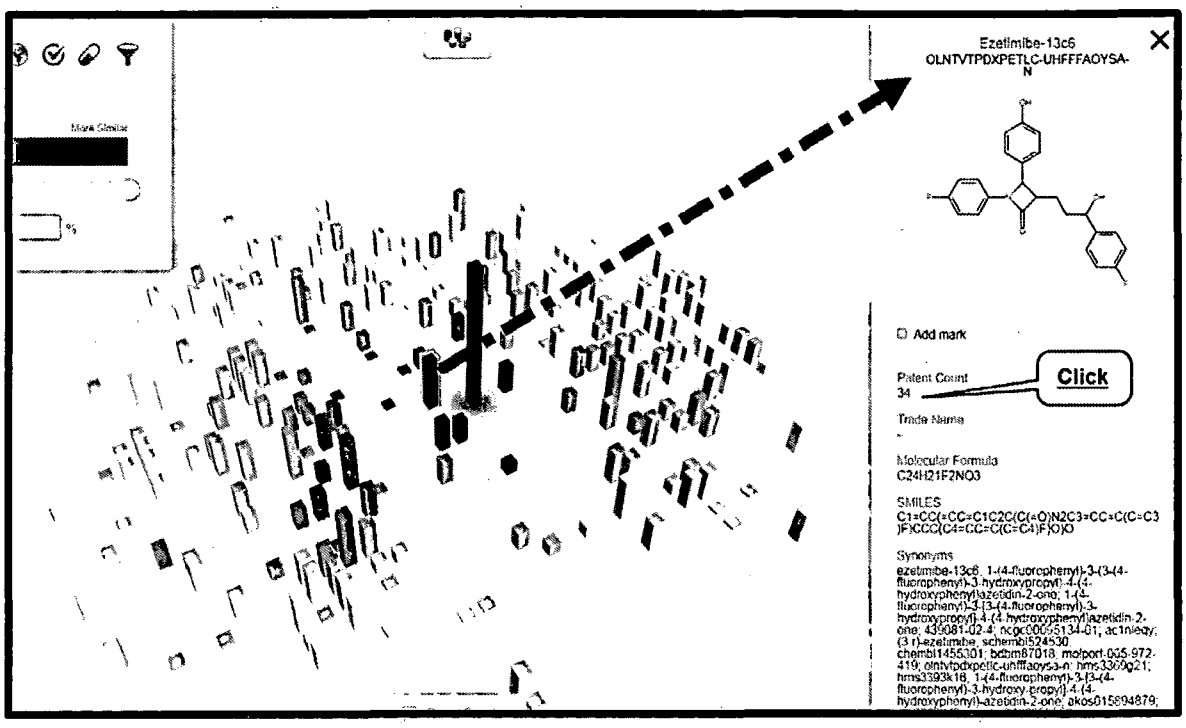
Select Structure
Save
ScreenShot

Fig. 31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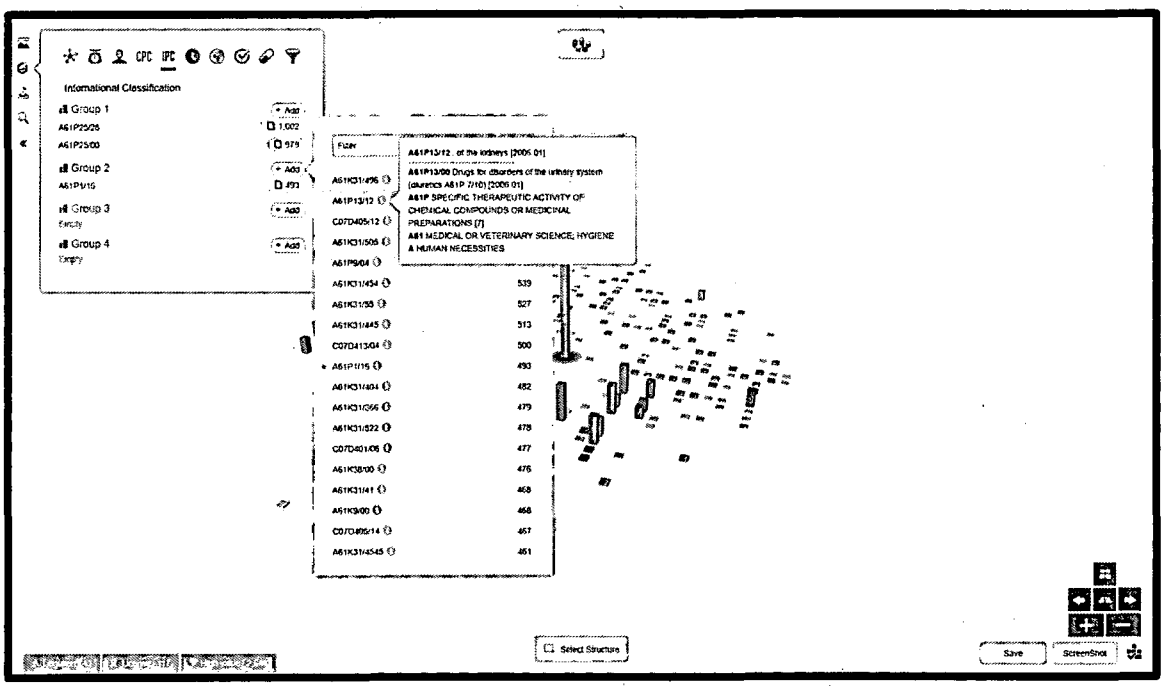
SMILES
Synonyms

Fig. 32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Group 2
Group 3
Group 4
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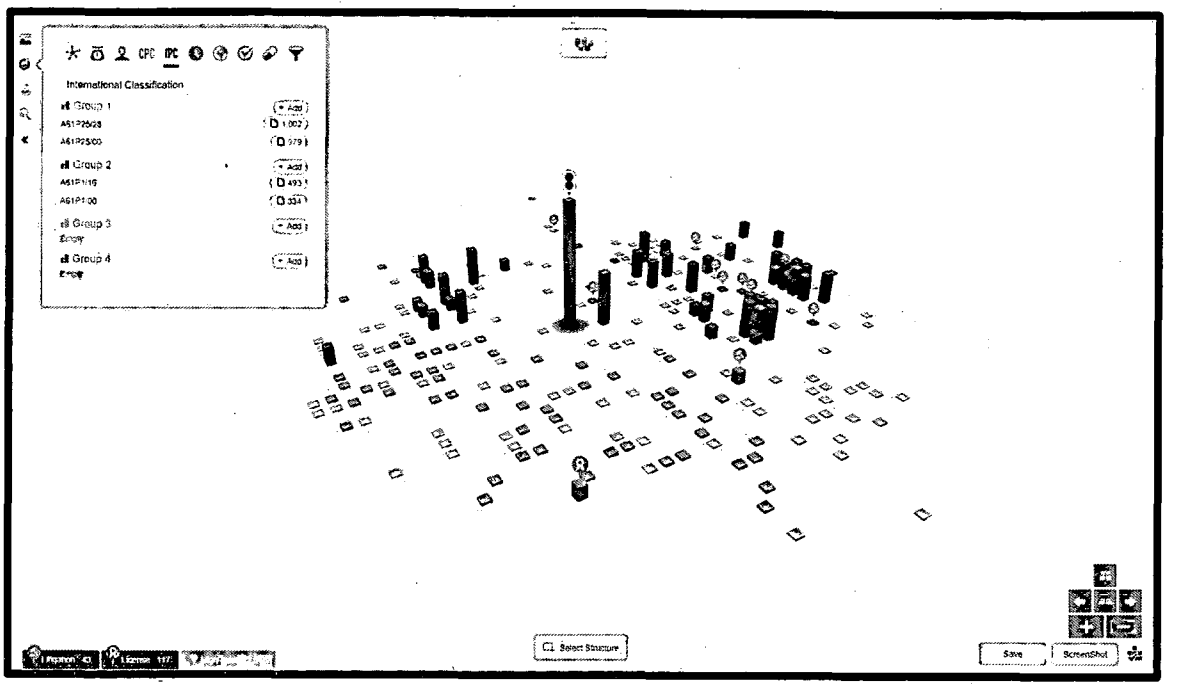
Save
ScreenShot

Fig. 33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Group 2
Group 3
Group 4
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Save
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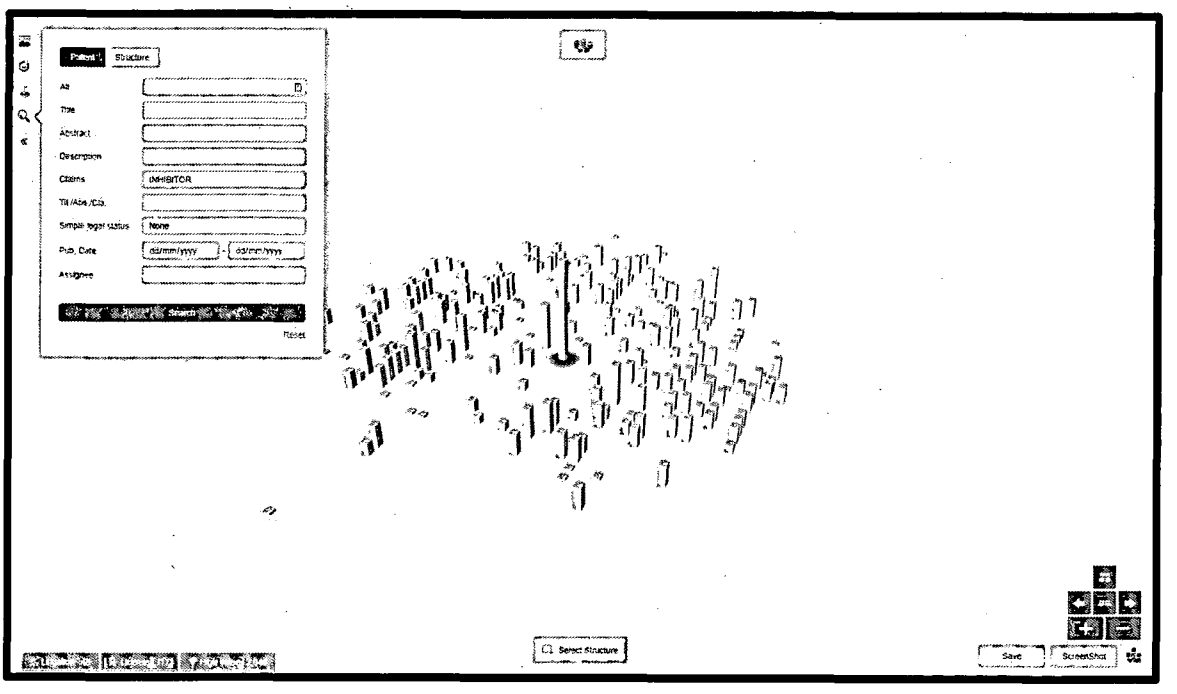
Fig. 34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Title
Abstract
Description
Claims
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Reset
Select Structure
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Fig. 35

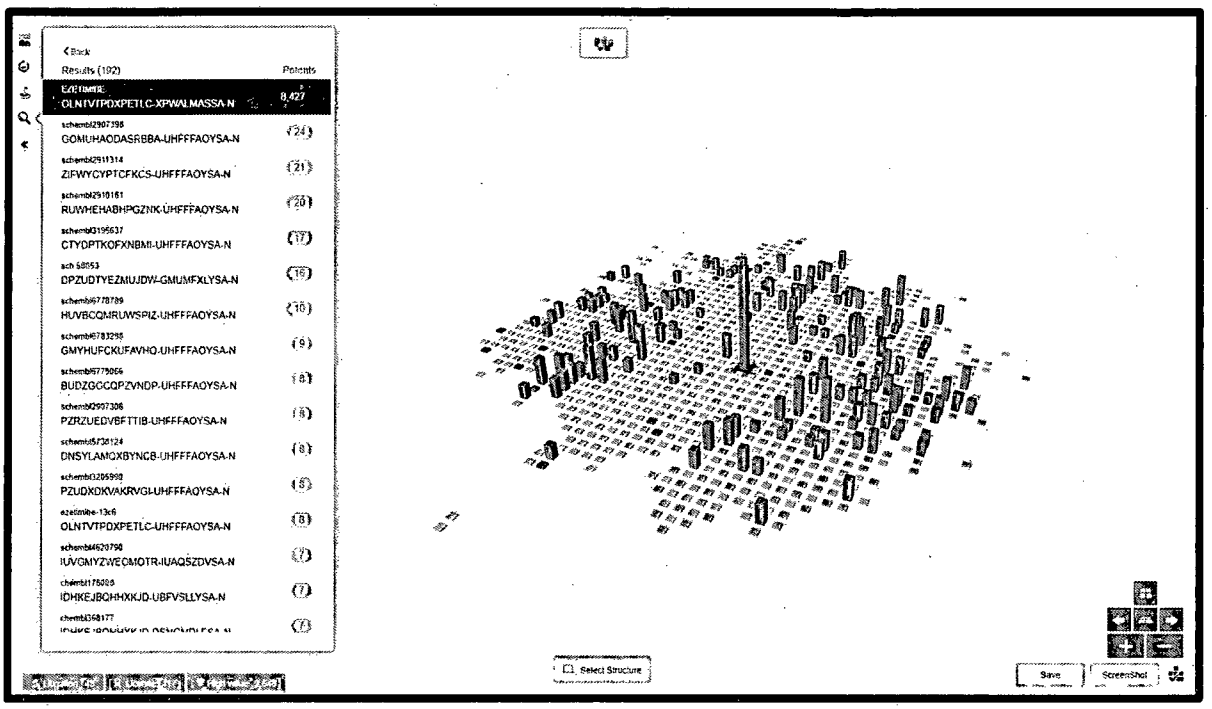
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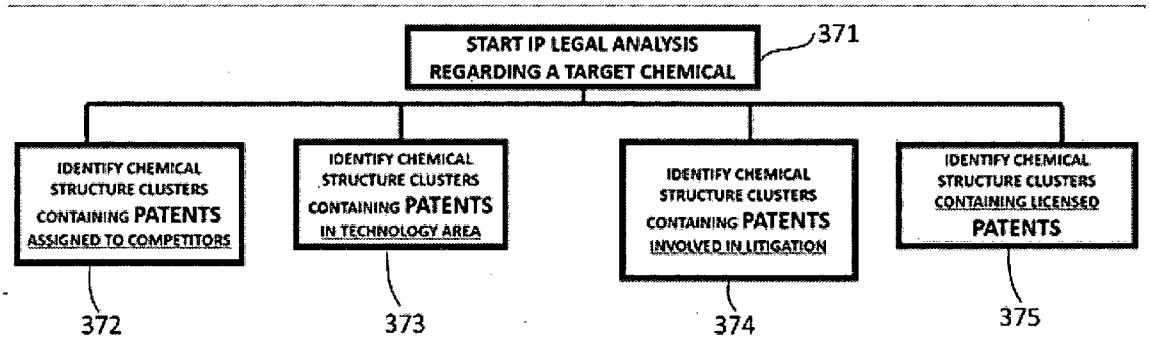
Fig. 36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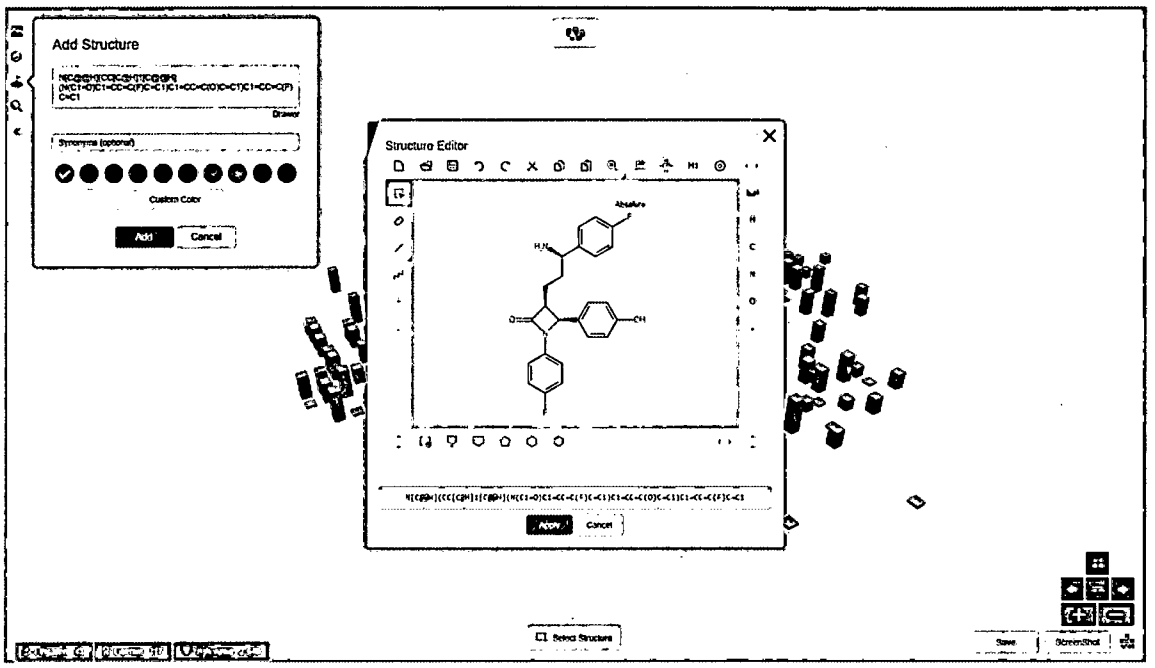
372
IDENTIFY CHEMICAL STRUCTURE CLUSTERS CONTAINING PATENTS IN TECHNOLOGY AREA
373
IDENTIFY CHEMICAL STRUCTURE CLUSTERS CONTAINING PATENTS INVOLVED IN LITIGATION
374
IDENTIFY CHEMICAL STRUCTURE CLUSTERS CONTAINING LICENSED PATENTS
375

Fig. 37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Drawer
Synonyms (optional)
Custom Color
Add
Cancel
Structure Editor
Apply
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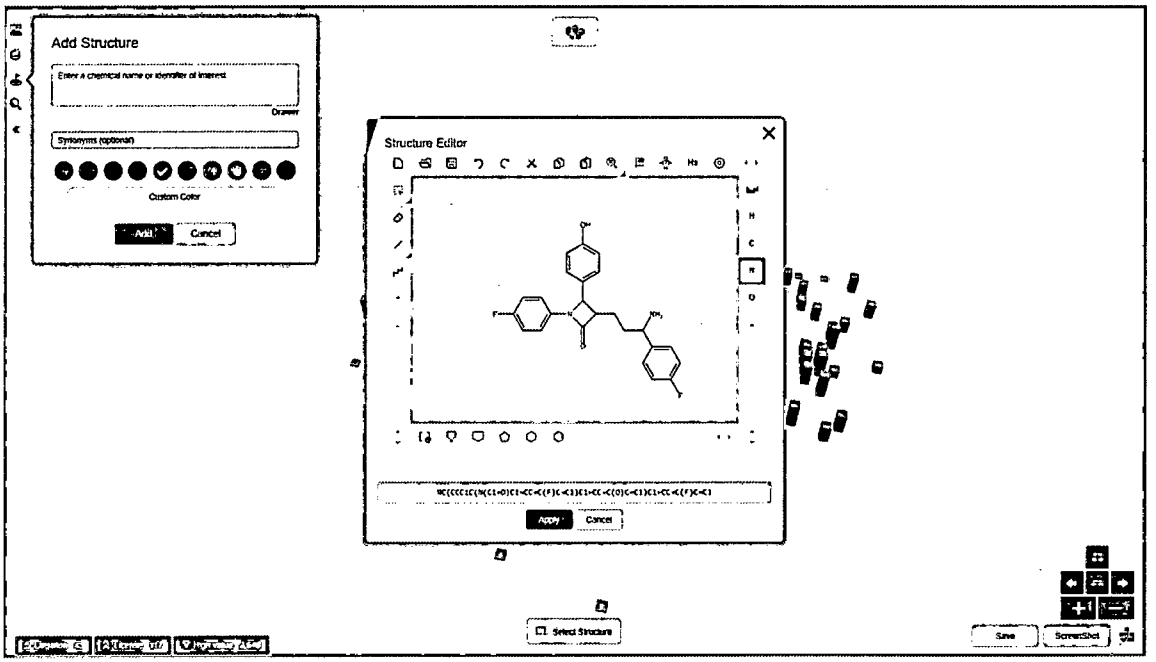
Select Structure
Save
ScreenShot

Fig. 38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Synonyms (optional)
Custom Color
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Apply
Cancel
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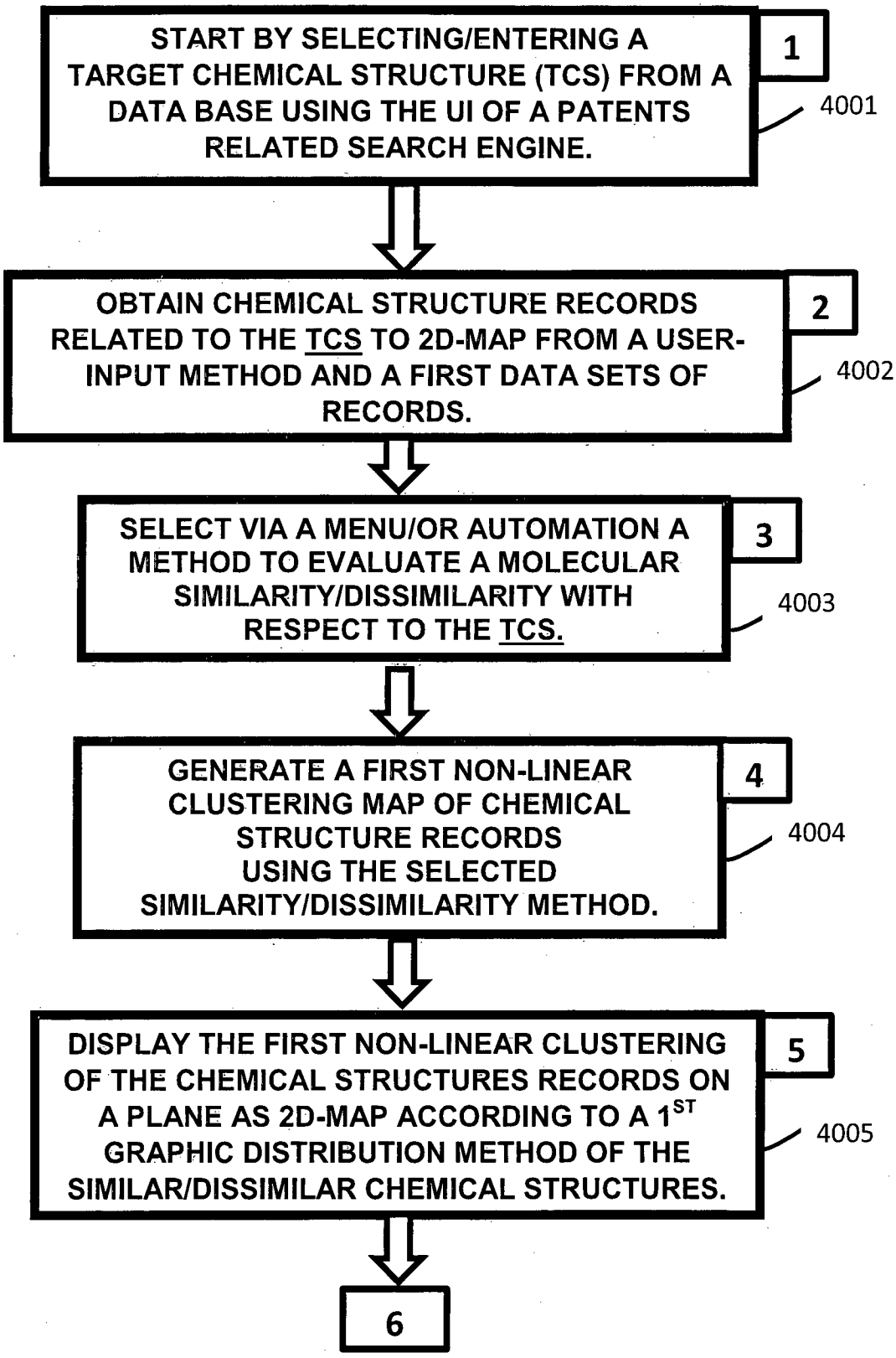
Save
ScreenShot

Fig. 39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OBTAIN CHEMICAL STRUCTURE RECORDS RELATED TO THE TCS TO 2D-MAP FROM A USER-INPUT METHOD AND A FIRST DATA SETS OF RECORDS.
2
4002
SELECT VIA A MENU/OR AUTOMATION A METHOD TO EVALUATE A MOLECULAR SIMILARITY/DISSIMILARITY WITH RESPECT TO THE TCS.
3
4003
GENERATE A FIRST NON-LINEAR CLUSTERING MAP OF CHEMICAL STRUCTURE RECORDS USING THE SELECTED SIMILARITY/DISSIMILARITY METHOD.
4
4004
DISPLAY THE FIRST NON-LINEAR CLUSTERING OF THE CHEMICAL STRUCTURES RECORDS ON A PLANE AS 2D-MAP ACCORDING TO A 1ST GRAPHIC DISTRIBUTION METHOD OF THE SIMILAR/DISSIMILAR CHEMICAL STRUCTURES.
5
4005
6

Fig. 40

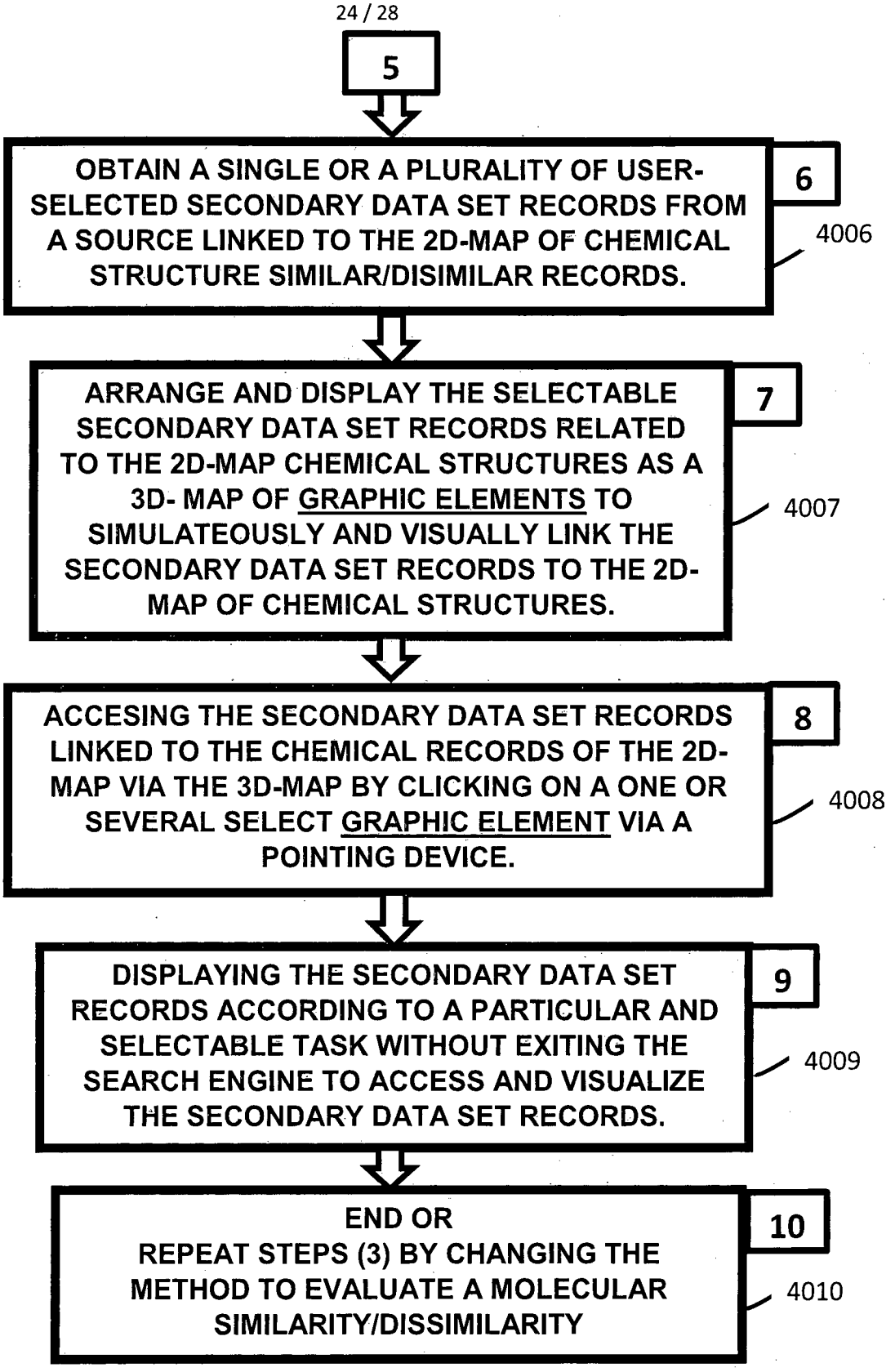
5
OBTAIN A SINGLE OR A PLURALITY OF USER-SELECTED SECONDARY DATA SET RECORDS FROM A SOURCE LINKED TO THE 2D-MAP OF CHEMICAL STRUCTURE SIMILAR/DISIMILAR RECORDS.
6
4006
ARRANGE AND DISPLAY THE SELECTABLE SECONDARY DATA SET RECORDS RELATED TO THE 2D-MAP CHEMICAL STRUCTURES AS A 3D- MAP OF GRAPHIC ELEMENTS TO SIMULATEOUSLY AND VISUALLY LINK THE SECONDARY DATA SET RECORDS TO THE 2D-MAP OF CHEMICAL STRUCTURES.
7
4007
ACCESING THE SECONDARY DATA SET RECORDS LINKED TO THE CHEMICAL RECORDS OF THE 2D-MAP VIA THE 3D-MAP BY CLICKING ON A ONE OR SEVERAL SELECT GRAPHIC ELEMENT VIA A POINTING DEVICE.
8
4008
DISPLAYING THE SECONDARY DATA SET RECORDS ACCORDING TO A PARTICULAR AND SELECTABLE TASK WITHOUT EXITING THE SEARCH ENGINE TO ACCESS AND VISUALIZE THE SECONDARY DATA SET RECORDS.
9
4009
END OR
REPEAT STEPS (3) BY CHANGING THE METHOD TO EVALUATE A MOLECULAR SIMILARITY/DISSIMILARITY
10
4010

Fig. 41

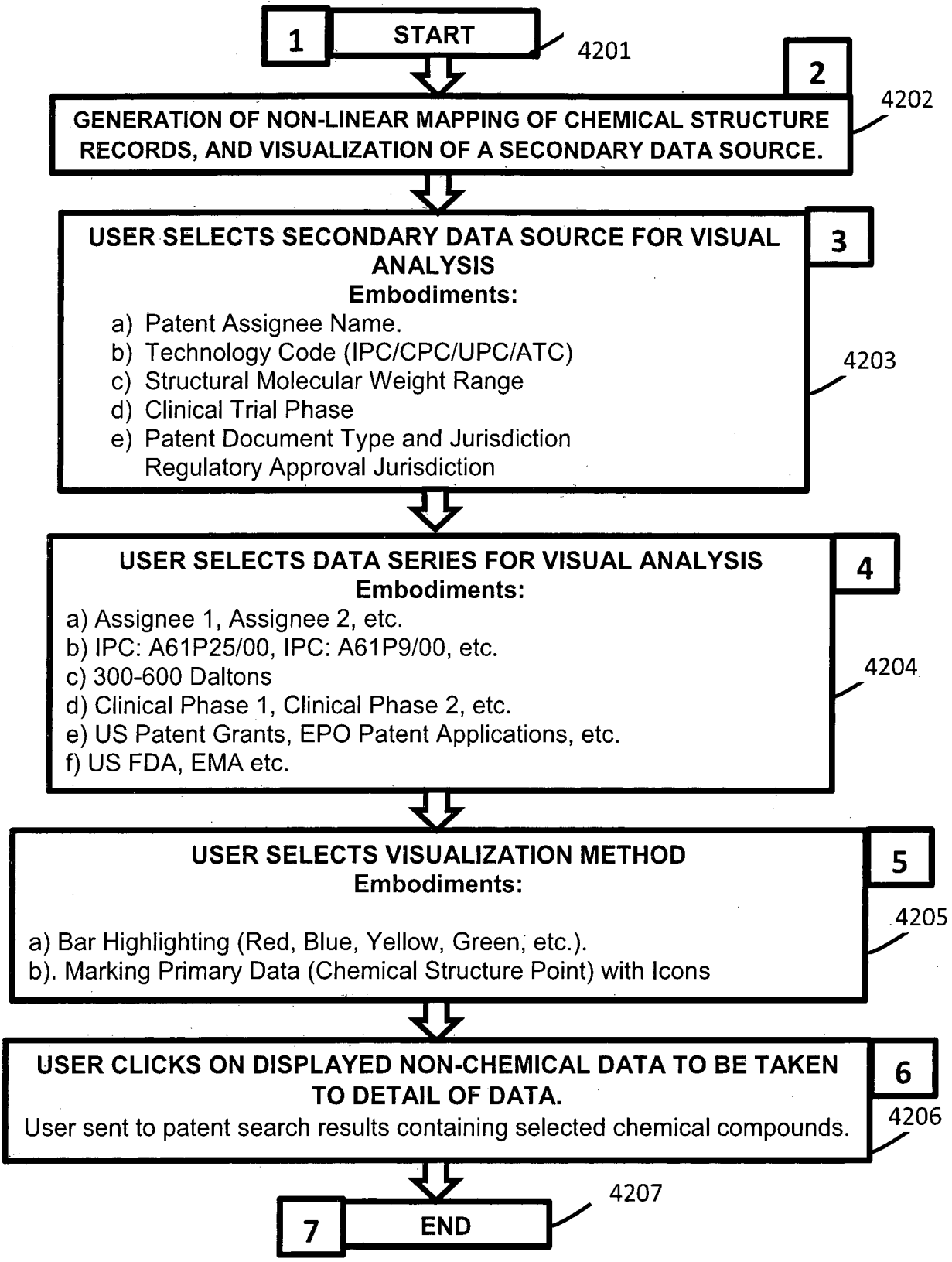
1
START
4201
2
GENERATION OF NON-LINEAR MAPPING OF CHEMICAL STRUCTURE RECORDS, AND VISUALIZATION OF A SECONDARY DATA SOURCE.
4202
USER SELECTS SECONDARY DATA SOURCE FOR VISUAL ANALYSIS
Embodiments:
a) Patent Assignee Name.
b) Technology Code (IPC/CPC/UPC/ATC)
c) Structural Molecular Weight Range
d) Clinical Trial Phase
e) Patent Document Type and Jurisdiction
Regulatory Approval Jurisdiction
3
4203
USER SELECTS DATA SERIES FOR VISUAL ANALYSIS
Embodiments:
a) Assignee 1, Assignee 2, etc.
b) IPC: A61P25/00, IPC: A61P9/00, etc.
c) 300-600 Daltons
d) Clinical Phase 1, Clinical Phase 2, etc.
e) US Patent Grants, EPO Patent Applications, etc.
f) US FDA, EMA etc.
4
4204
USER SELECTS VISUALIZATION METHOD
Embodiments:
a) Bar Highlighting (Red, Blue, Yellow, Green, etc.).
b). Marking Primary Data (Chemical Structure Point) with Icons
5
4205
USER CLICKS ON DISPLAYED NON-CHEMICAL DATA TO BE TAKEN TO DETAIL OF DATA.
User sent to patent search results containing selected chemical compounds.
6
4206
7
END
4207

Fig. 42

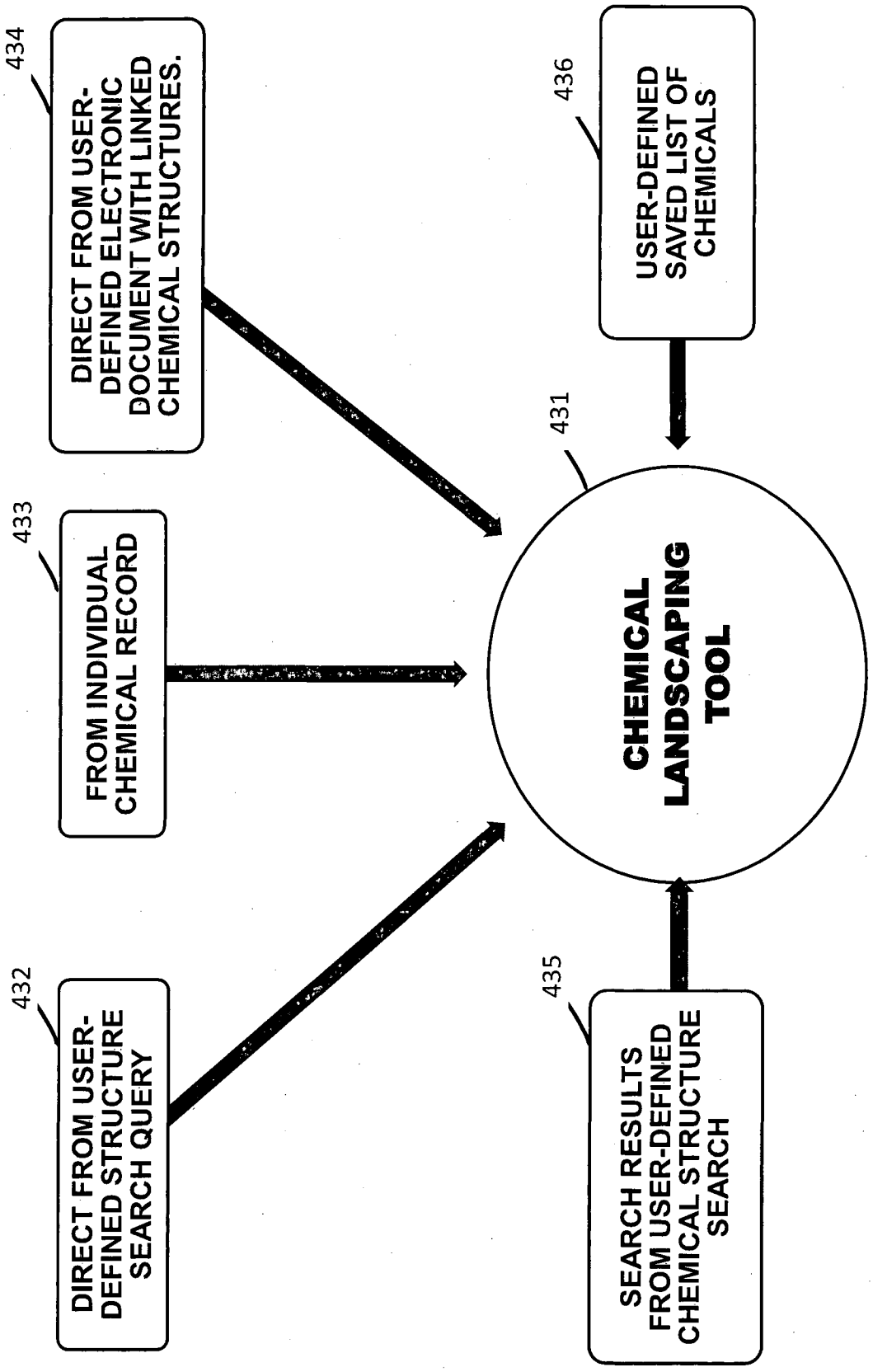
CHEMICAL LANDSCAPING TOOL
431
DIRECT FROM USER-DEFINED ELECTRONIC DOCUMENT WITH LINKED CHEMICAL STRUCTURES.
434
FROM INDIVIDUAL CHEMICAL RECORD
433
DIRECT FROM USER-DEFINED STRUCTURE SEARCH QUERY
432
USER-DEFINED SAVED LIST OF CHEMICALS
436
SEARCH RESULTS FROM USER-DEFINED CHEMICAL STRUCTURE SEARCH
435

Fig. 43

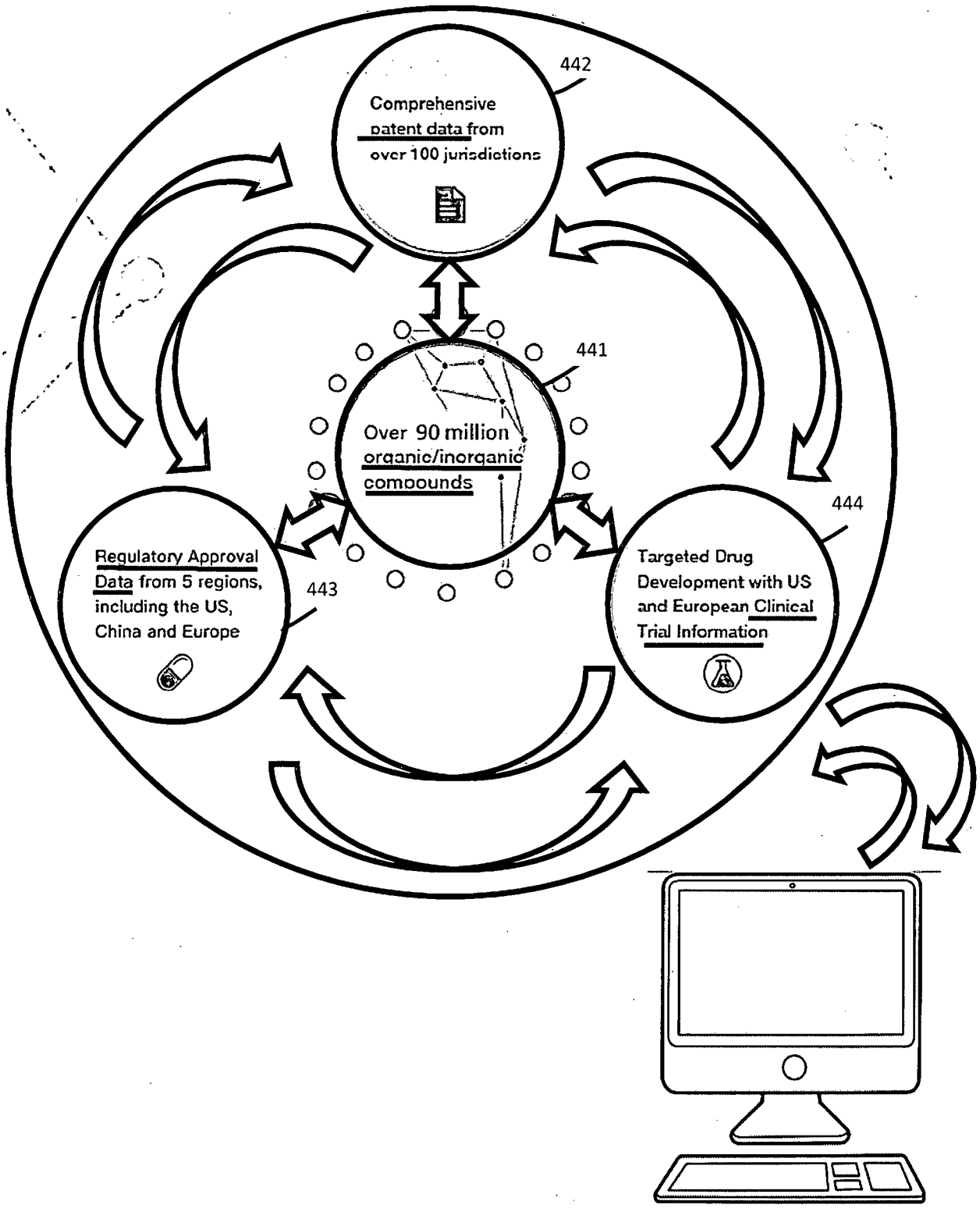
442
Comprehensive patent data from over 100 jurisdictions
441
Over 90 million organic/inorganic compounds
443
Regulatory Approval Data from 5 regions, including the US, China and Europe
444
Targeted Drug Development with US and European Clinical Trial Information

Fig. 44

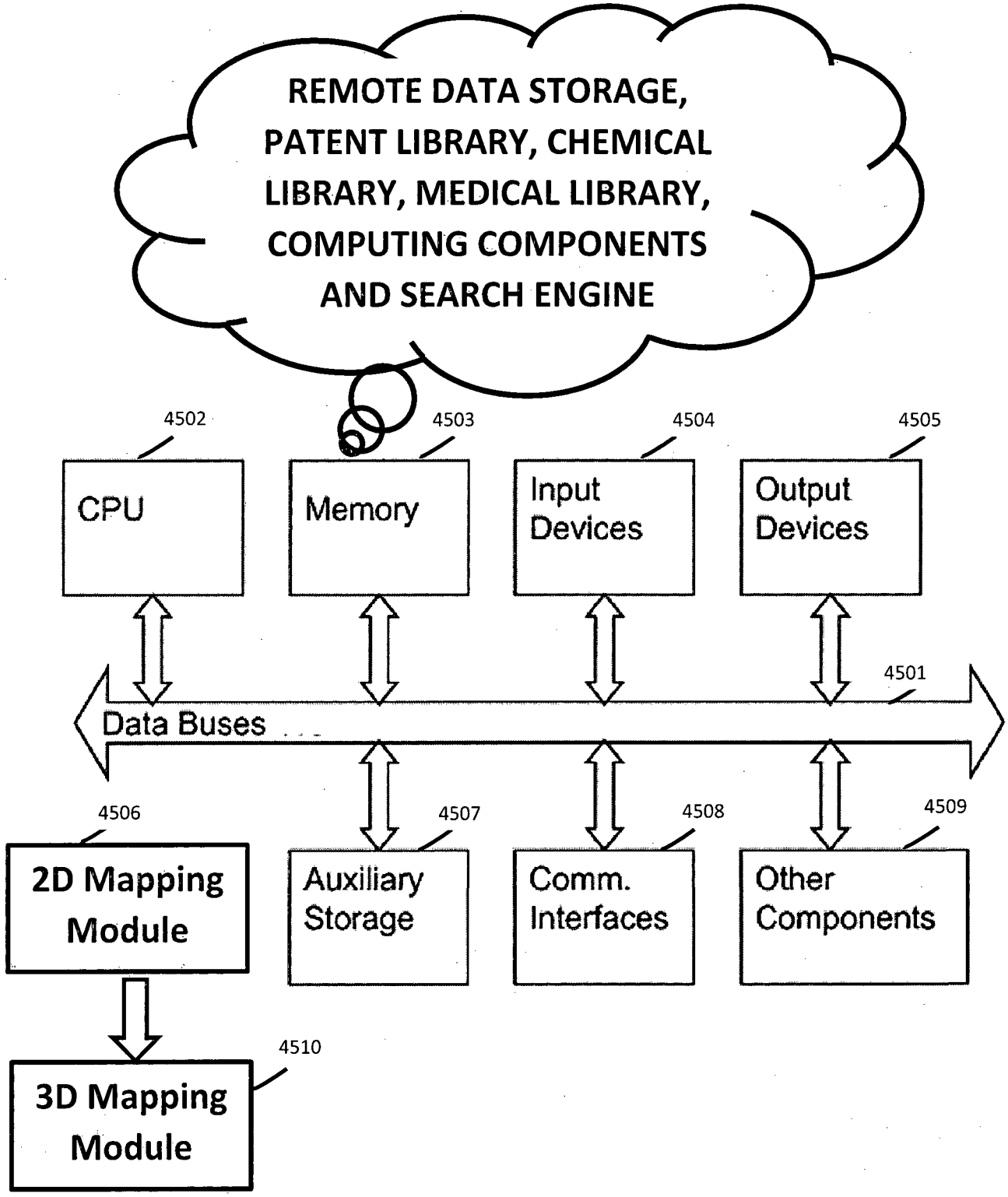
REMOTE DATA STORAGE, PATENT LIBRARY, CHEMICAL LIBRARY, MEDICAL LIBRARY, COMPUTING COMPONENTS AND SEARCH ENGINE
4502
CPU
4503
Memory
4504
Input Devices
4505
Output Devices
4501
Data Buses
4506
2D Mapping Module
4507
Auxiliary Storage
4508
Comm. Interfaces
4509
Other Components
4510
3D Mapping Module

Fig. 45

INTERNATIONAL SEARCH REPORT

International application No.
PCT/CN2017/114656

A. CLASSIFICATION OF SUBJECT MATTER

G06F 17/30(2006.01)i

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPI,EPODOC,CNPAT,CNKI,IEEE:chemical w structure+, data w base, search+, patent+, map+, similar+

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	US 2013218878 A1 (CAMBRIDGESOFT CORPORATION) 22 August 2013 (2013-08-22) paragraphs [0035]-[0065],figures 2-3	1-4
A	US 2014372448 A1 (AMERICAN CHEMICAL SOCIETY) 18 December 2014 (2014-12-18) the whole document	1-4
A	CN 102929907 A (SHANGHAI TITAN TECHNOLOGY CO.,LTD.) 13 February 2013 (2013-02-13) the whole document	1-4
A	CN 105069155 A (CHANGSHA LUZHI INFORMATION TECHNOLOGY CO.,LTD.) 18 November 2015 (2015-11-18) the whole document	1-4

☐ Further documents are listed in the continuation of Box C.

☑ See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
07 February 2018	**24 February 2018**

Name and mailing address of the ISA/CN	Authorized officer
STATE INTELLECTUAL PROPERTY OFFICE OF THE P.R.CHINA **6, Xitucheng Rd., Jimen Bridge, Haidian District, Beijing 100088** **China**	**YANG,Yingying**
Facsimile No. **(86-10)62019451**	Telephone No. **(86-10)01053961527**

INTERNATIONAL SEARCH REPORT
Information on patent family members

International application No.
PCT/CN2017/114656

Patent document cited in search report			Publication date (day/month/year)	Patent family member(s)			Publication date (day/month/year)
US	2013218878	A1	22 August 2013	EP	2567338	A1	13 March 2013
				AU	2011248243	A1	22 November 2012
				US	2011276589	A1	10 November 2011
				CA	2798294	A1	10 November 2011
				WO	2011140148	A1	10 November 2011
				HK	1183350	A0	20 December 2011
US	2014372448	A1	18 December 2014	WO	2014201402	A1	18 December 2014
CN	102929907	A	13 February 2013		None		
CN	105069155	A	18 November 2015		None		