CAS SciFinder^{n}

Search Guide

August 2021

https://scifinder-n.cas.org/

CAS
A division of the
American Chemical Society

JAICI
化学情報協会

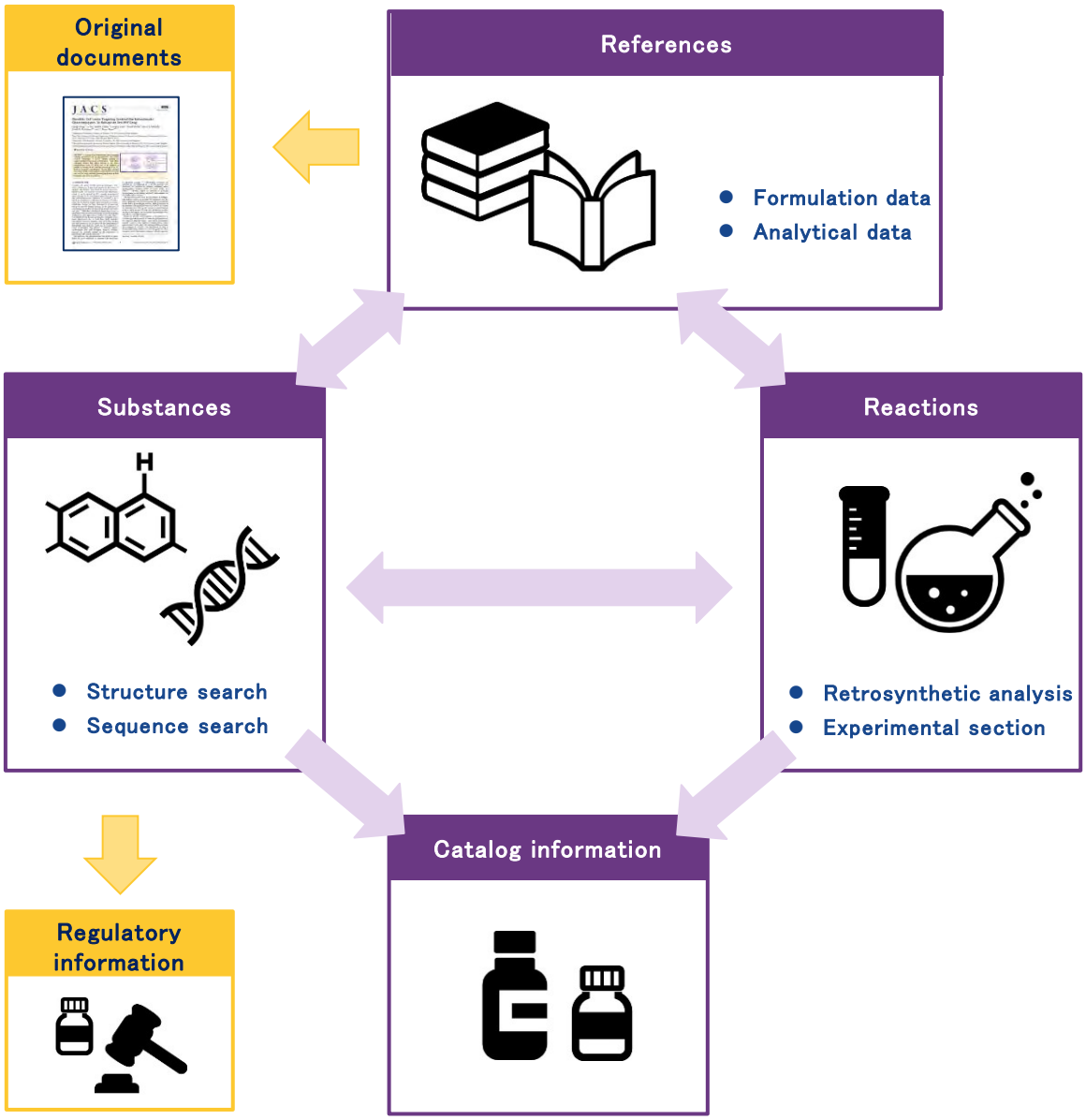
Features in CAS SciFinder^{n}

■ CAS SciFinder^{n} is an online search tool for CAS databases designed for researchers.

- Contain scientific information such as references, substances, reactions and so on
- Access to the largest substance database containing all CAS RN®*
  * CAS RN® is a unique and unambiguous identifier for a specific substance
- Suitable for searching information on scientific area
- Used globally by companies or main scientific faculties in universities (science, technology, pharmacy, agriculture, etc)

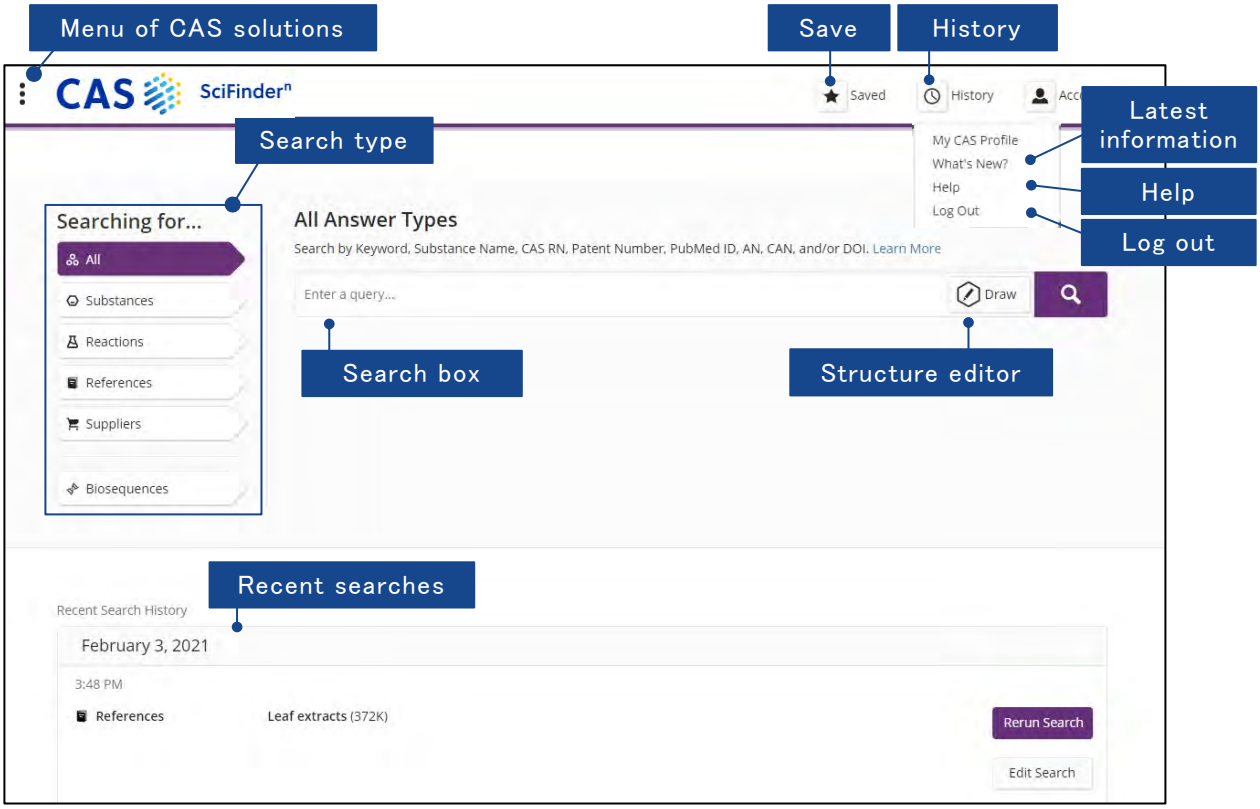
■ You can search references, substances, reactions, and catalog information in CAS SciFinder^{n}

- Each information is linked through CAS Registry Number (CAS RN®)



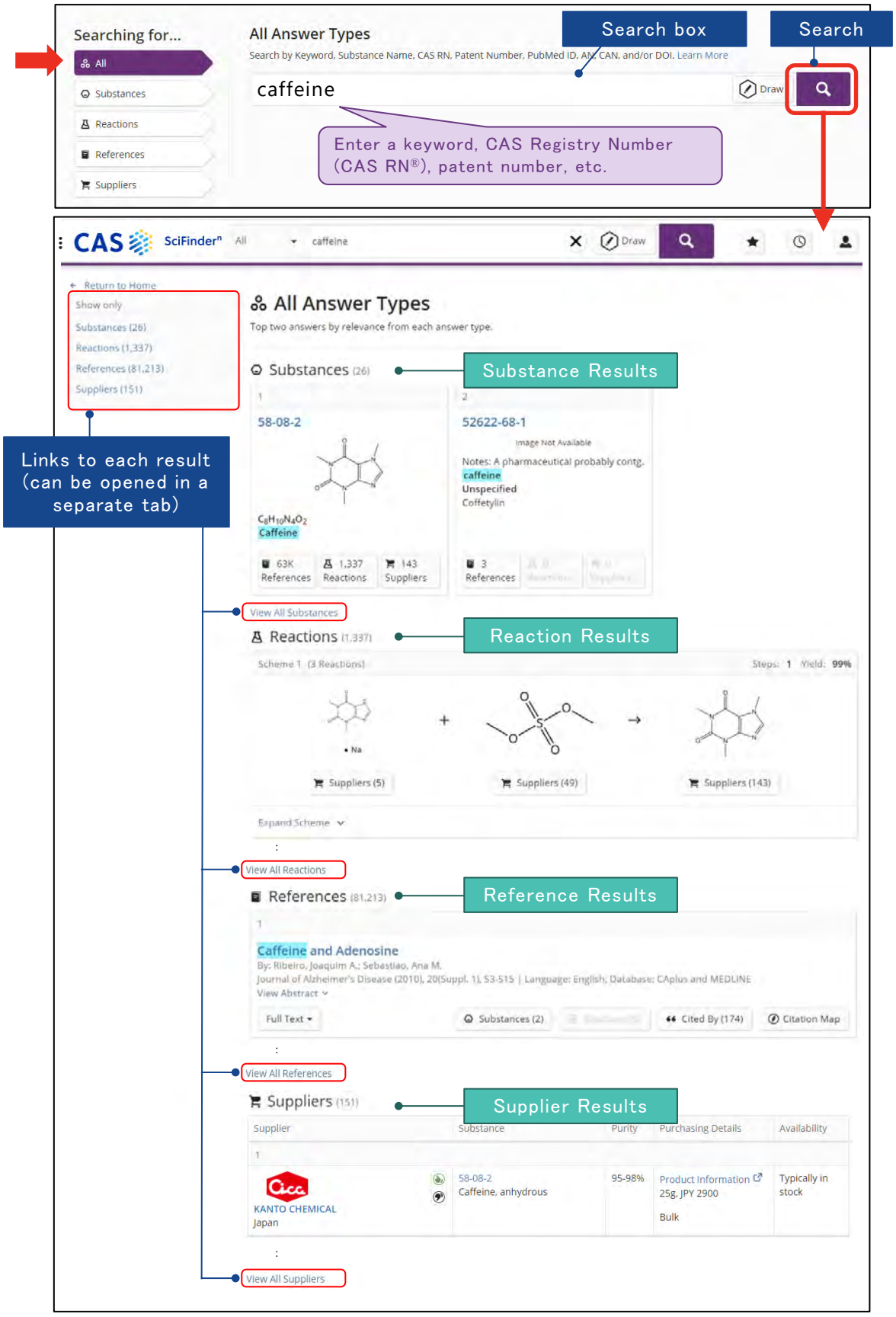
Home page

■ Top of the Home page



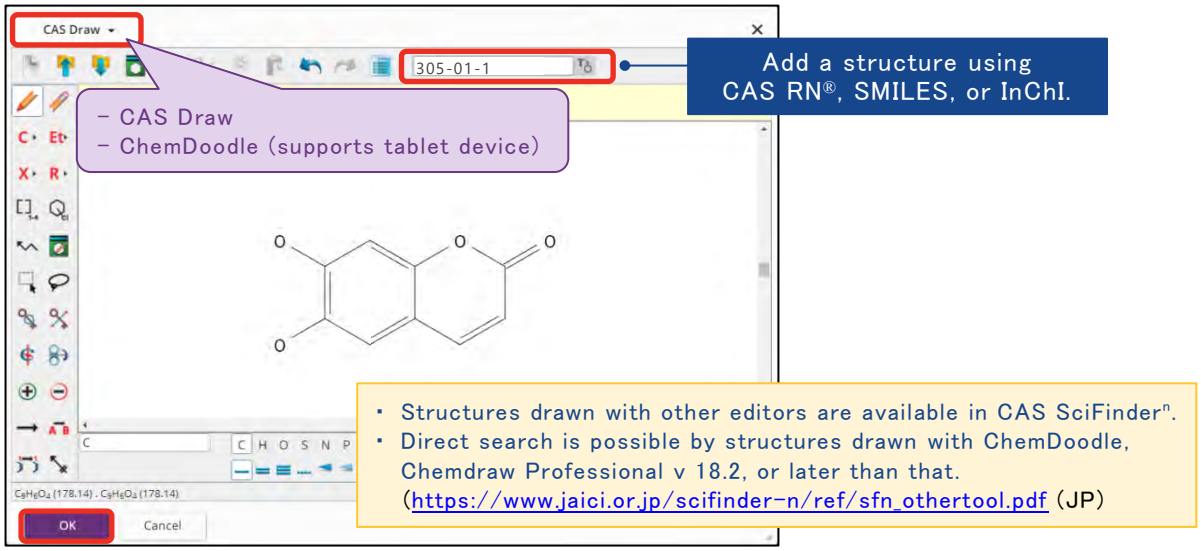
All search

■ All finds substances, reactions, references, and suppliers that match your query.



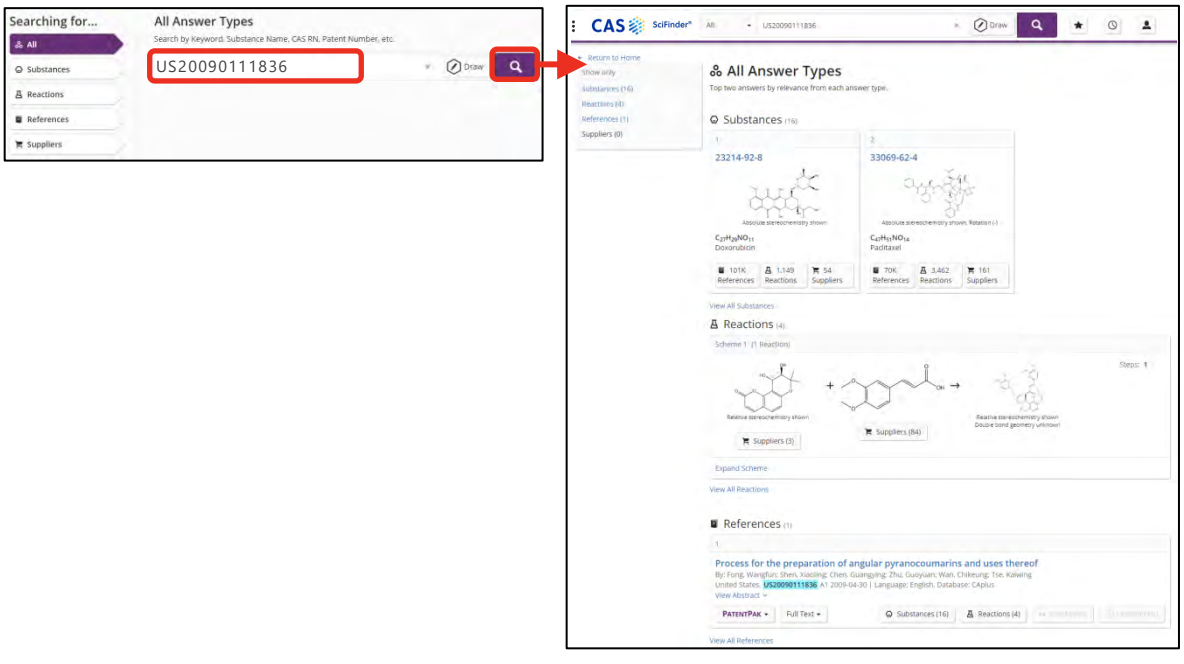
■ To search by chemical structure, click the Draw button and draw a structure.

・ You can select CAS Draw or ChemDoodle.



・ Click the Search button.

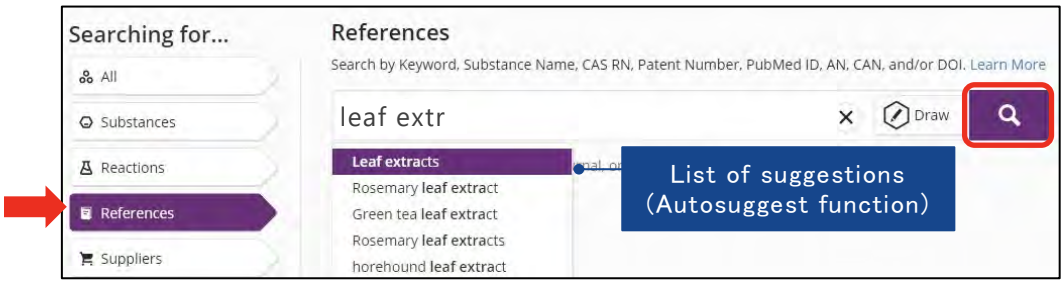
■ Searching a patent number in All search retrieves substances and reactions mentioned in the patent in addition to its patent record..



Reference search

■ In the Reference search, you can find references by keyword, author name, journal information (journal name, volume number, issue number, etc.), organization or document identifier.

・ Keyword and Document Identifier (Patent Number, DOI, Accession Number, etc.)



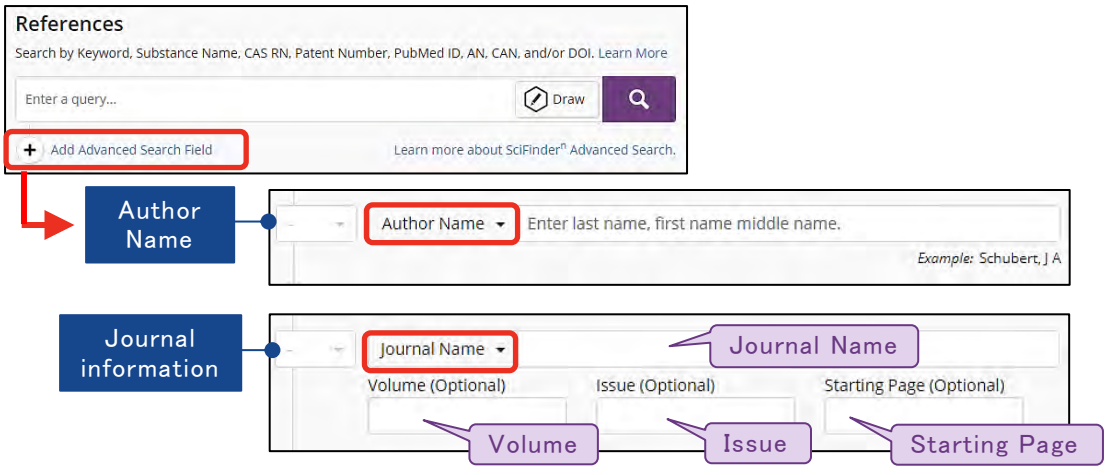
– Boolean search operators (AND, OR, NOT) or wildcards (*, ?) are available when combining keywords (See www.jaici.or.jp/scifinder-n/ref/sfn_boolean.pdf.).

– The main search field searches title, abstract, indexing, and document identifier. If you search terms in other information or choose a field to search, please see below.

・ Author name, Journal Information and Organization

– You can combine multiple author names, journal information, organization, etc.

– Click Add Advanced Search Field and choose a field to search.



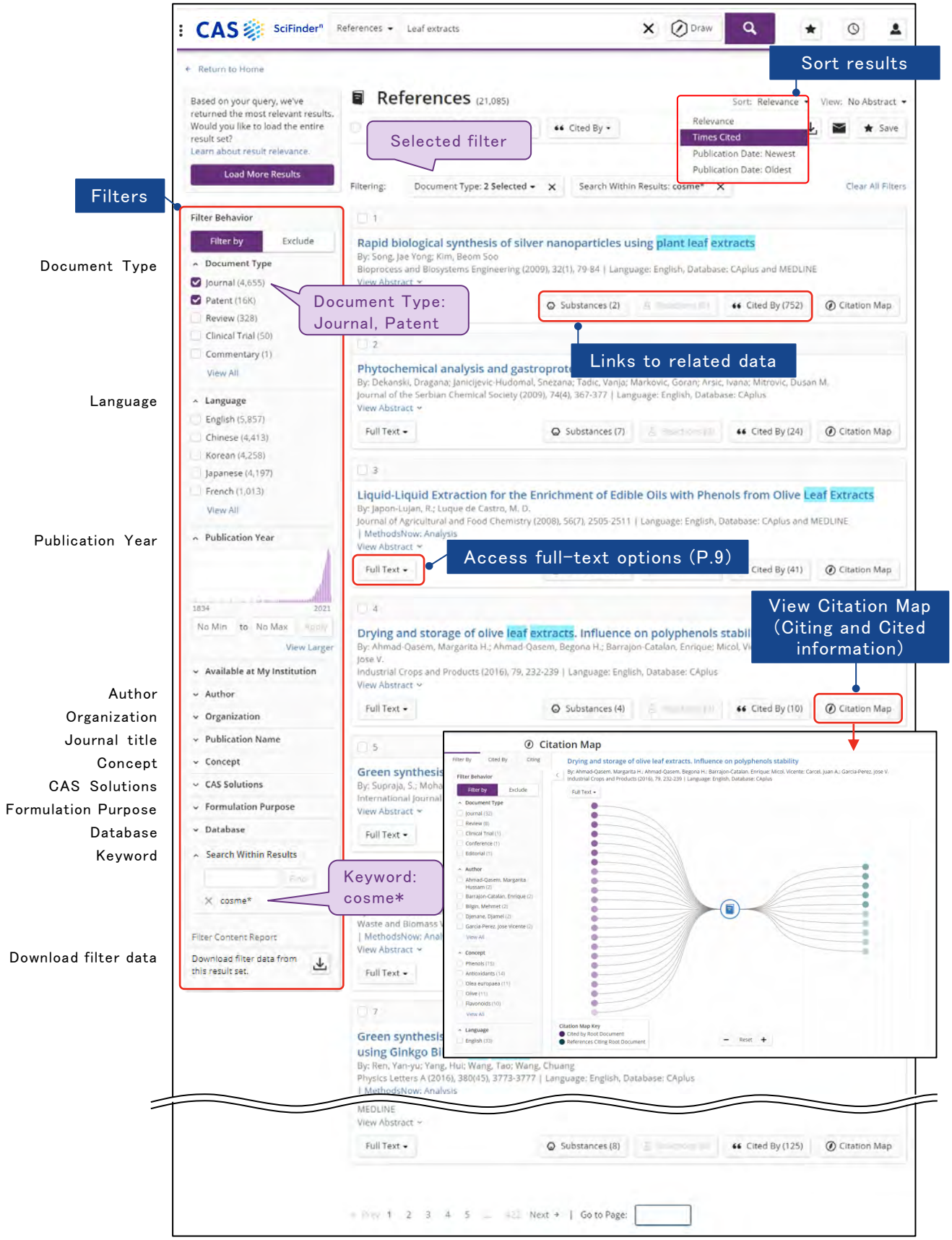
– Click Add Advanced Search Field and choose OR operator when combining multiple author names, journal information and organizations.

・ You can combine the main search field and Add Advanced Search Fields.

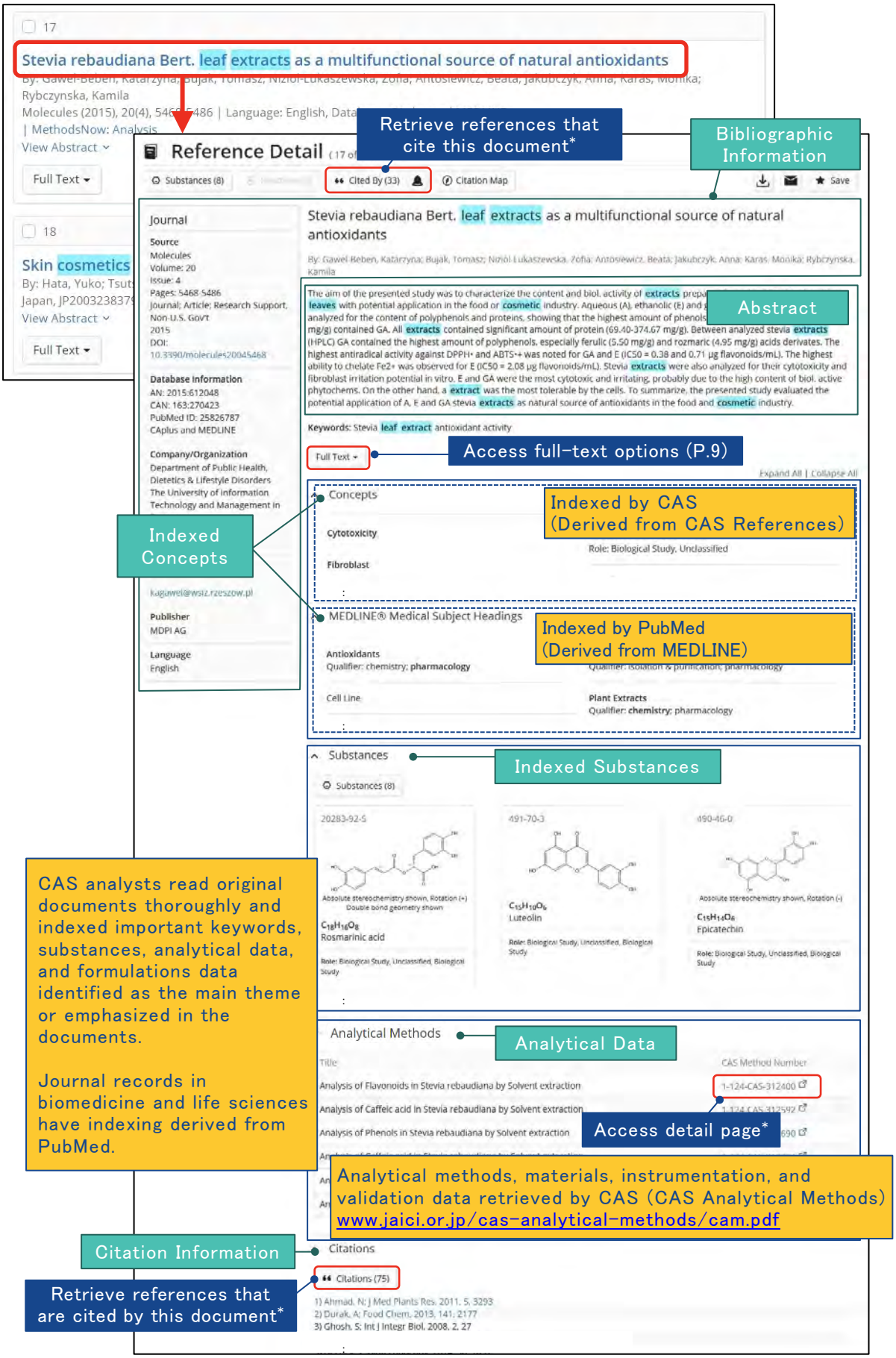
■ Answers are sorted by Relevance by default.

・ You can select other sort orders with Sort menu.

■ Select filers to display or exclude answers that match the applied filters.

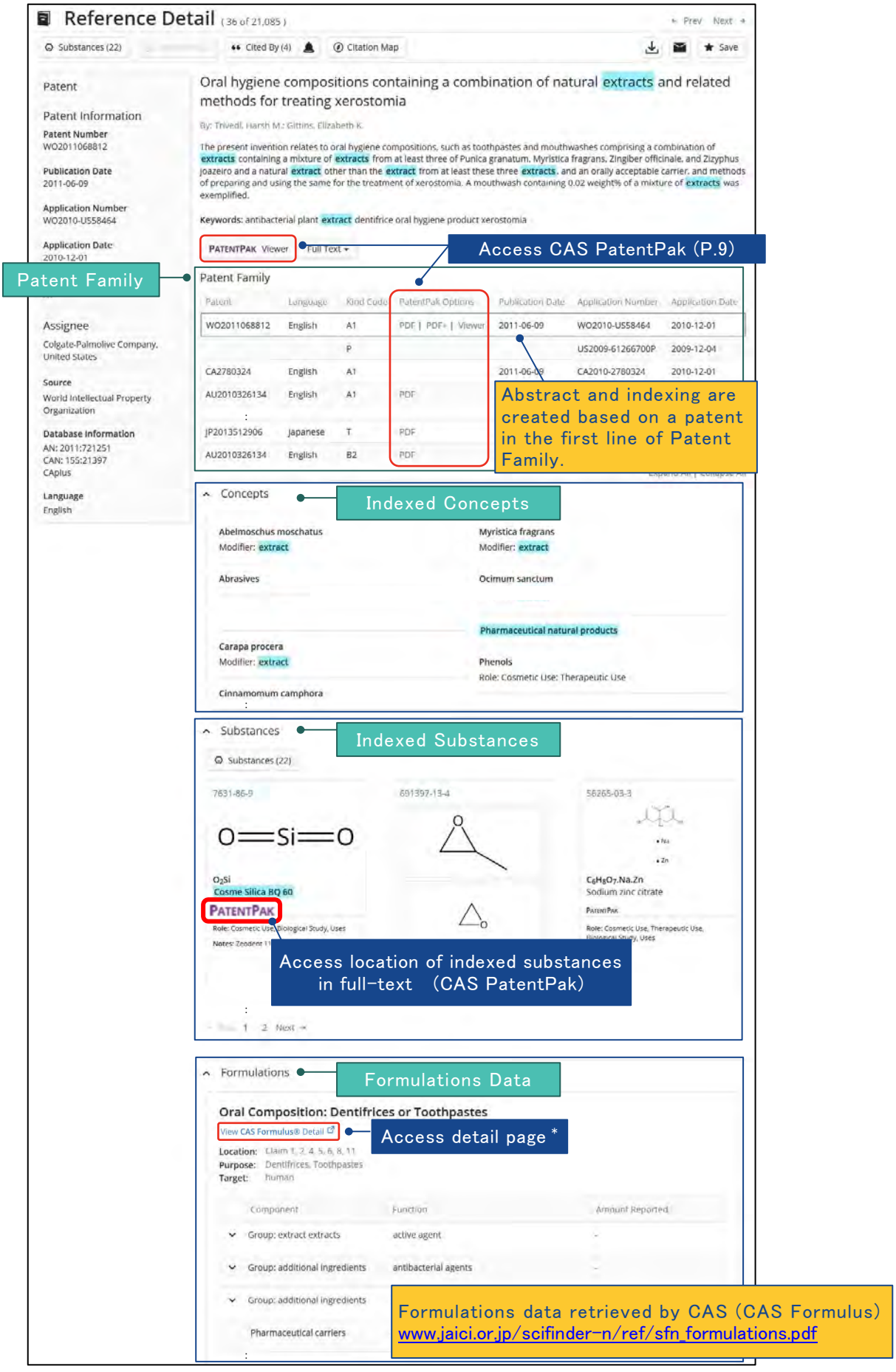


- To open the Reference Detail page, click the title.



* For the detail of citation searching with CAS SciFinder^{n}, see www.jaici.or.jp/scifinder-n/ref/sfn_citation.pdf.

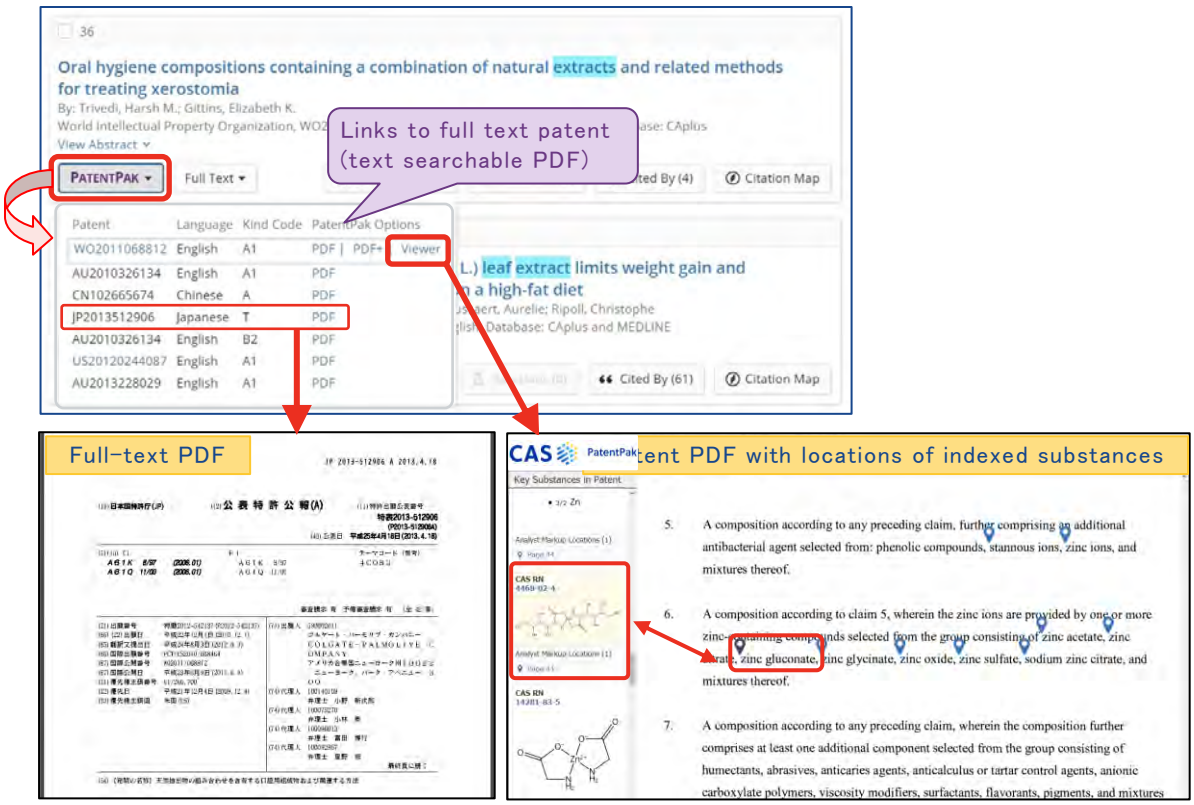
- Patent record



* Only those who make a contract for companies or government research institutions can access CAS Formulus and CAS Analytical Methods.

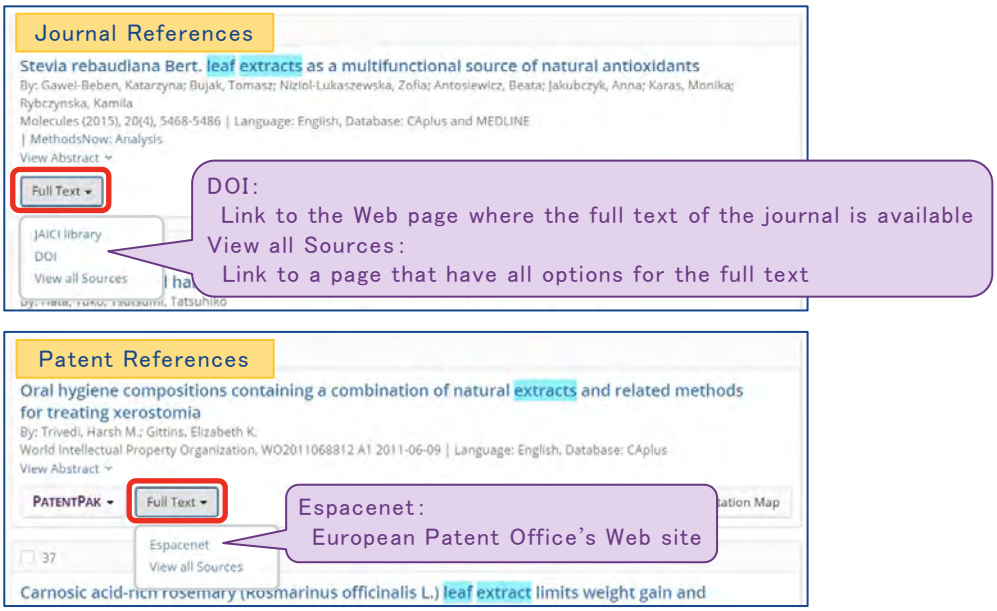
Access full text (CAS PatentPak, Full Text)

■ To access patent PDF with locations of indexed substances, click Viewer in PatentPak menu (See https://www.jaici.or.jp/scifinder-n/ref/sfn_pat.pdf).



■ To view full-text options for a reference, click the Full Text button and then select one of the following options.

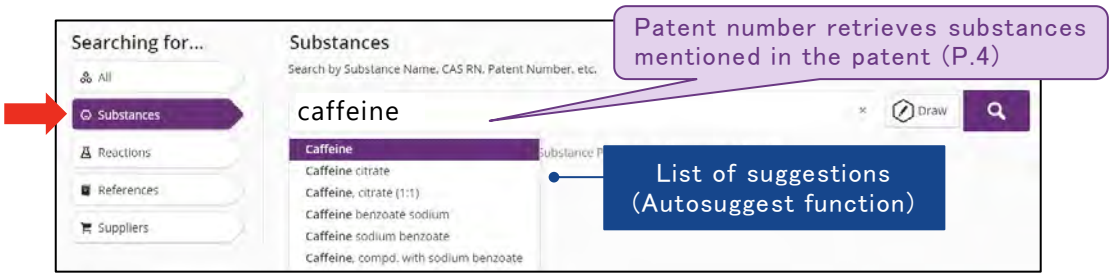
・ Selecting View all Sources opens a page that have all options for the full text.



Substance search

■ In the Substance search, you can find substances by substance name, chemical structure, CAS Registry Number (CAS RN®), molecular formula, etc.

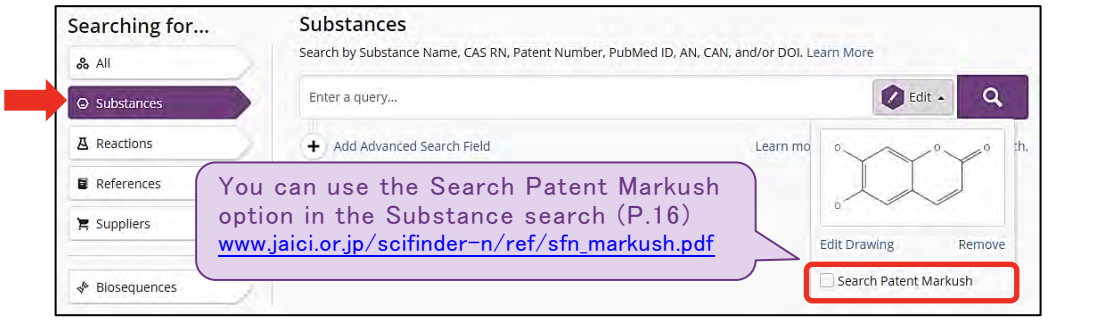
- Substance Name and CAS Registry Number (CAS RN®)



  - When entering multiple CAS RN®s or substance names, they must be separated by a space, no commas or other punctuation.

  - Substance name can search Notes in substance records with no structure information.

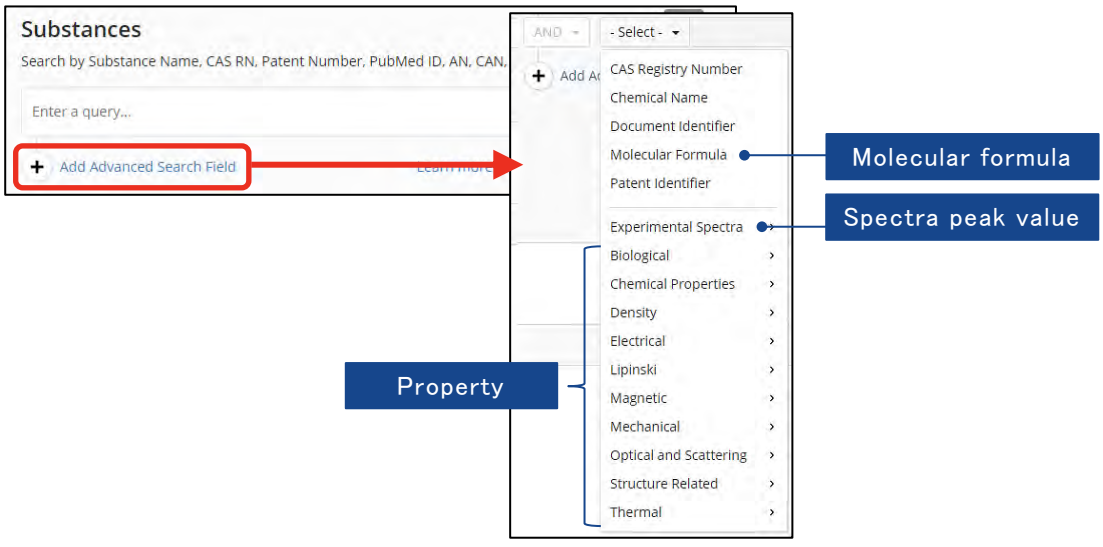
- Chemical Structure



  - To find patents by Markush structure, check the box for Search Patent Markush (P.16).

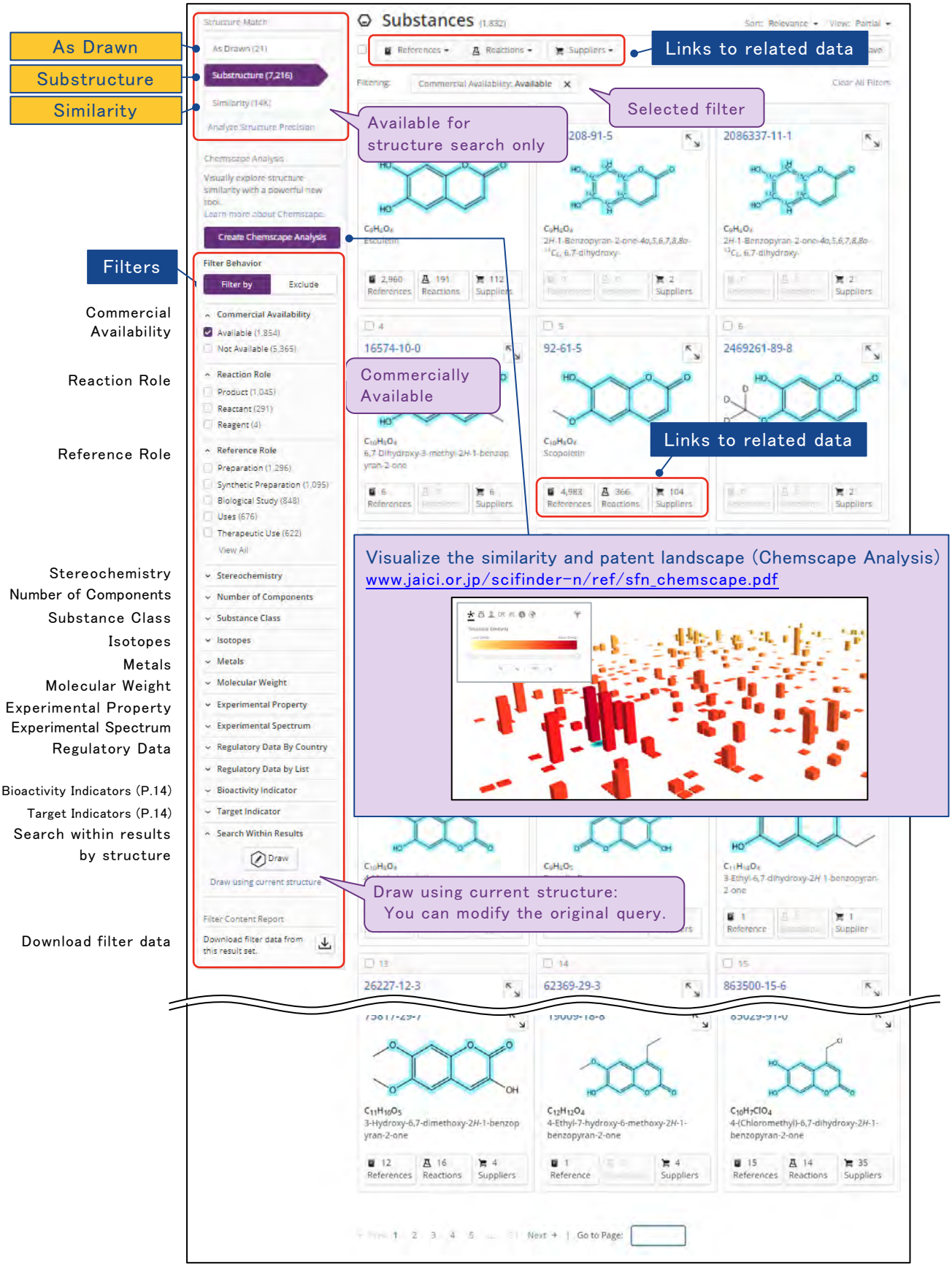
- Molecular Formula, Substance Property and Experimental Spectra

  - Click Add Advanced Search Field and select a field in the drop-down menu.

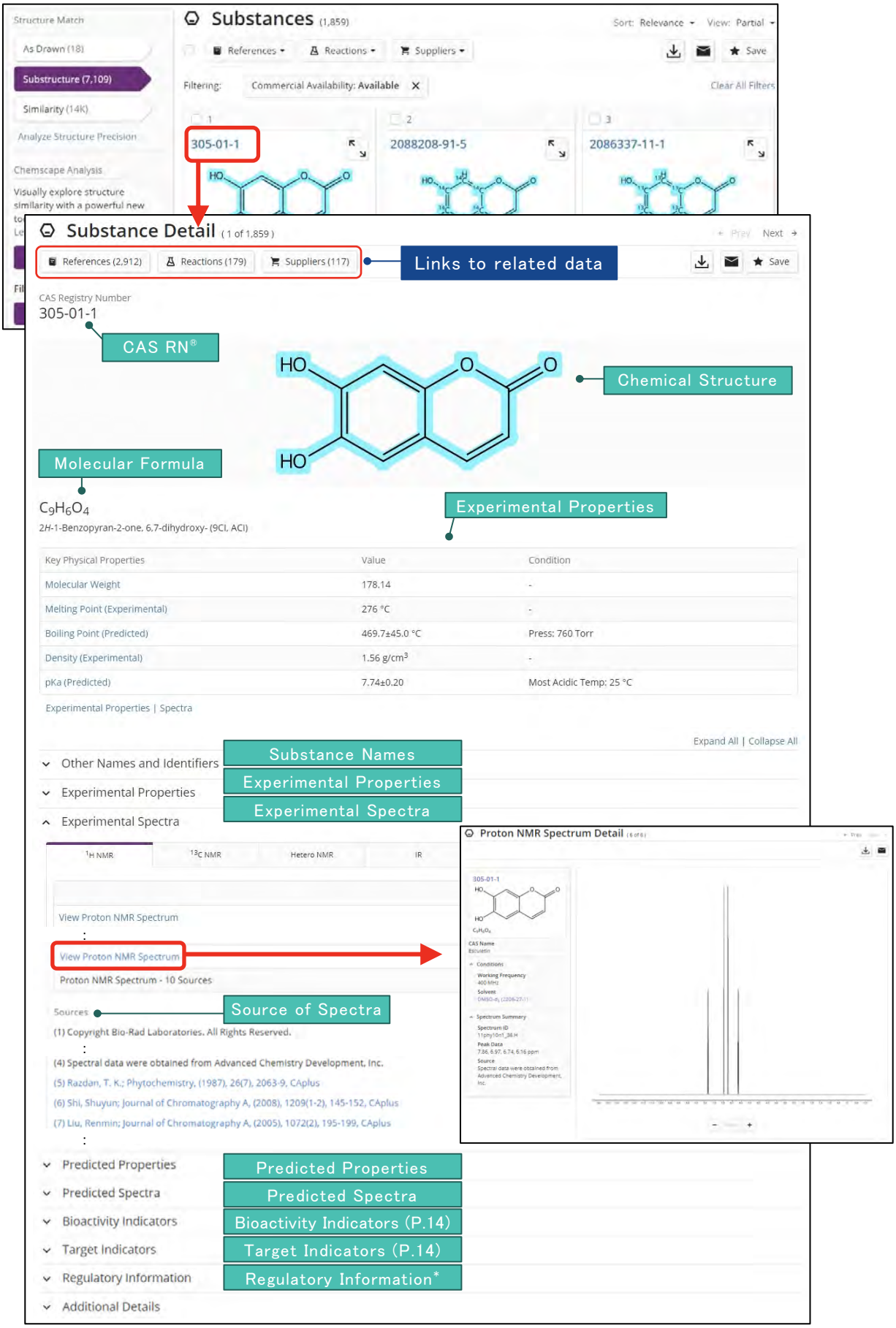


■ Select filers to display or exclude answers that match the applied filters.

- In chemical structure search, you can select the type of structure match.
  (See P.15 for the difference of each type)

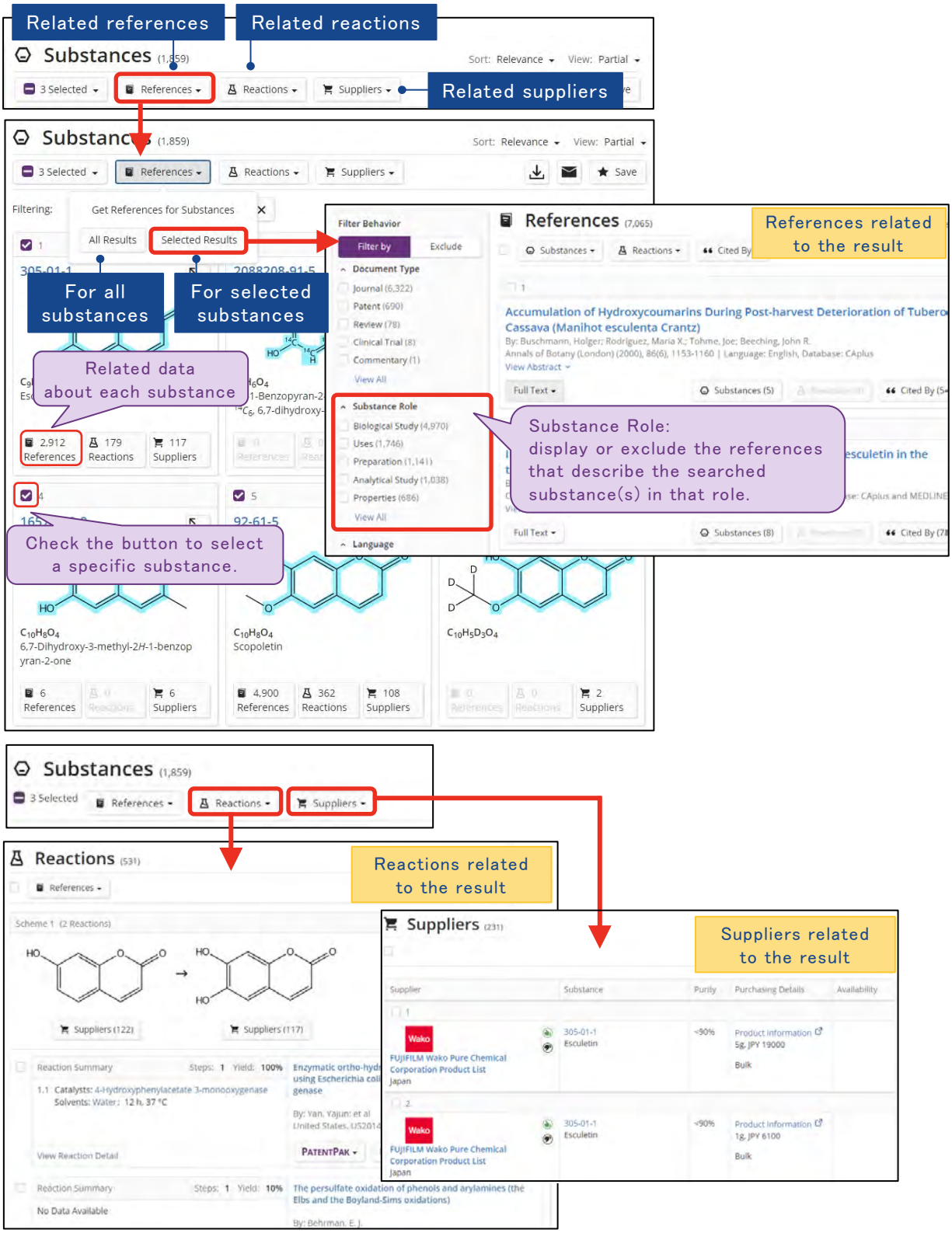


・ To open the Substance Detail page, click the CAS RN®.



* For the detail of regulatory information in CAS SciFinder^{n}, see www.jaici.or.jp/scifinder-n/ref/sfn_regulatory.pdf.

- You may retrieve data related to all or specific Substance page results.
  - To retrieve data about all substance results, click the All Results button.
  - To retrieve data about specific substance results, check the box for each substance, and then click the Selected Results button.



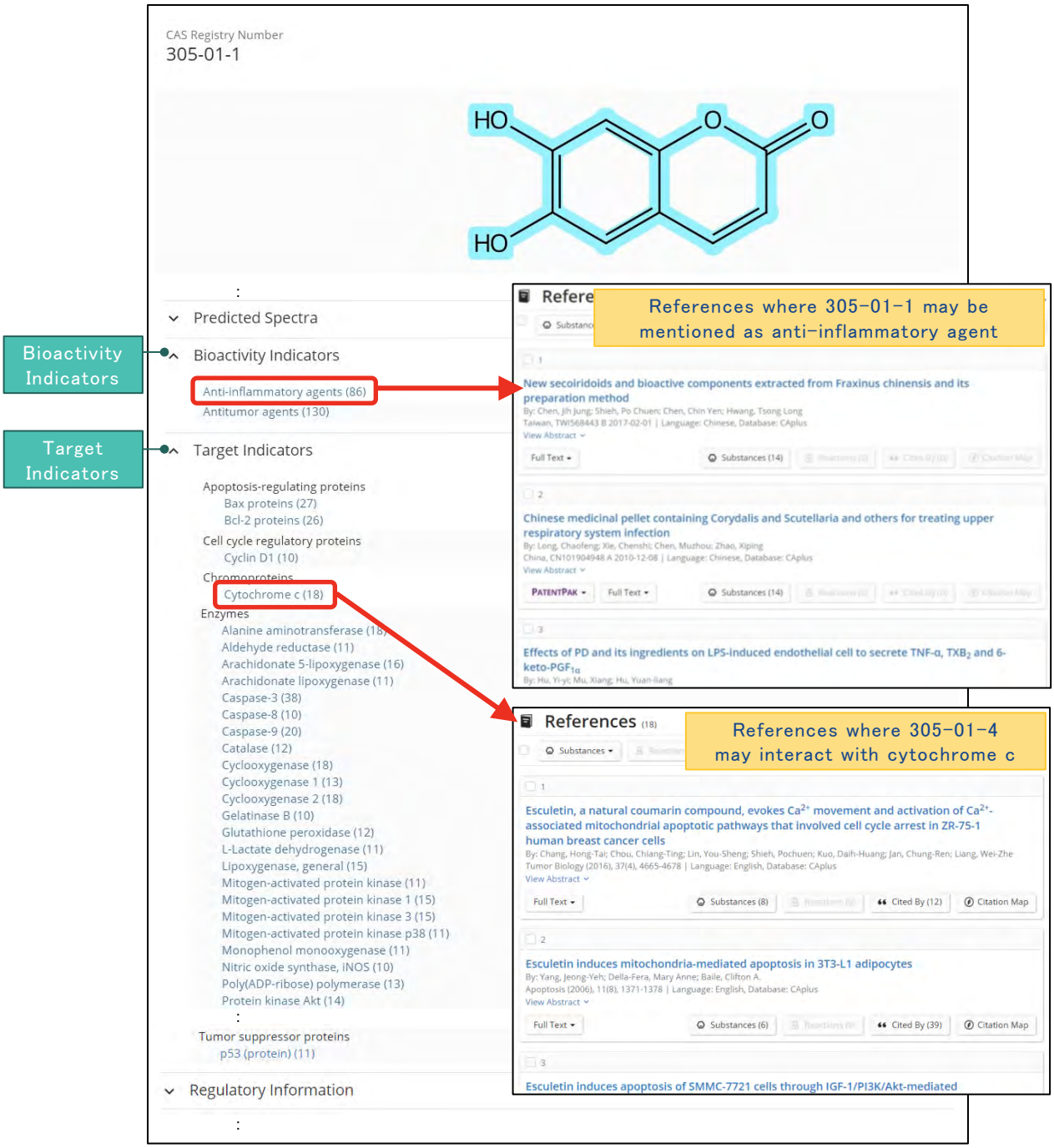
Tips: Bioactivity Indicators and Target Indicators

- Some substance records have Bioactivity Indicator and/or Target Indicators.

  - Bioactivity Indicators shows types of biological activity that substances in the result set may have.
    Example: Antitumor agents, Anti Platelet agents, etc.

  - Target Indicators shows types of receptors or enzymes that substances are expected to interact with.
    Example: α-amylase, dopamine receptor, etc.

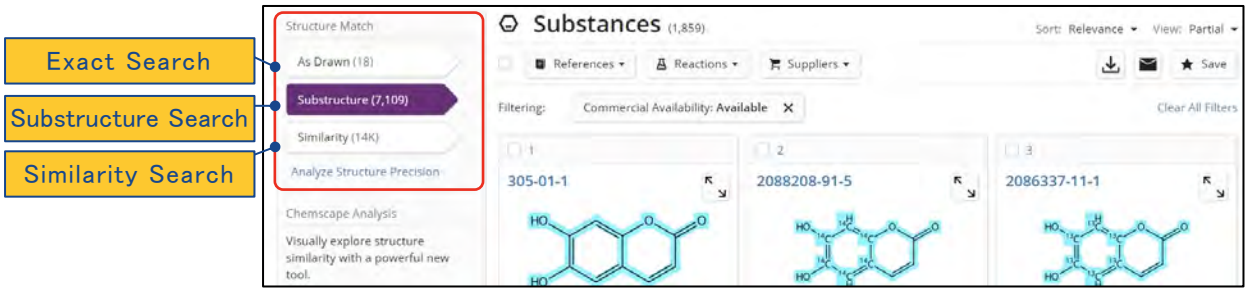
  - You can retrieve the references studying bioactivities, receptors, or enzymes related to the substance by clicking a link of each indicator name.



Tips: Chemical structure search type

■ Substances that match following three types will be retrieved automatically if you use a structure query.

・ Select the type you wish to view from Structure Match.

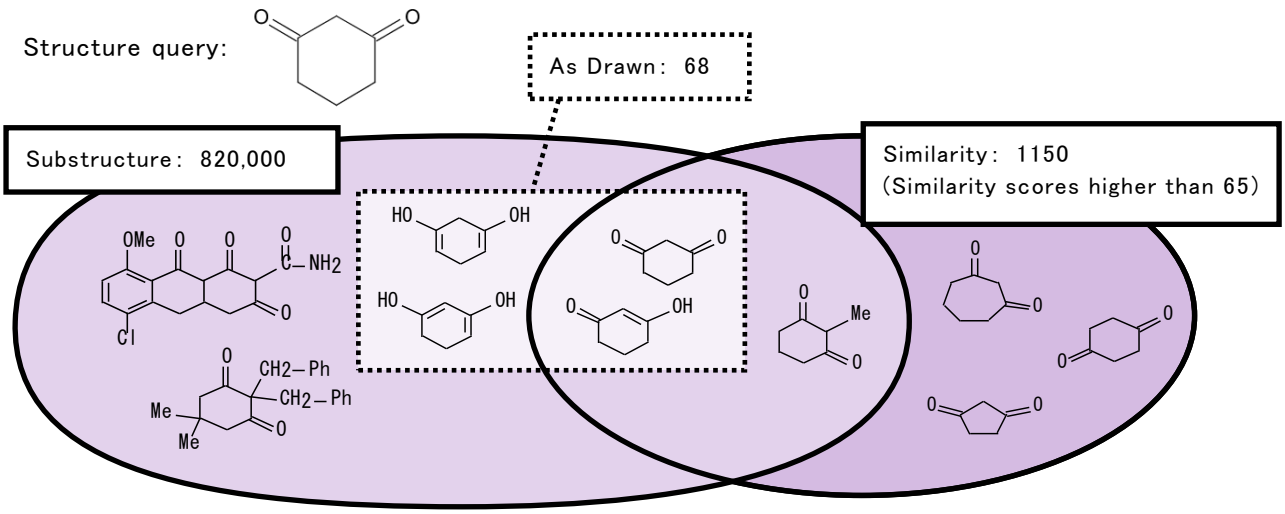


■ Difference in each search type

Search Type	Retrieved substances
As Drawn (Exact Search)	・**Substances that match the structure exactly as drawn** (including stereoisomers or isotopes) and multicomponent substances in which the queried structure appears ・Tautomers
Substructure (Substructure Search)	・In addition to the substances in a As drawn match, **any substituent is allowed at any open atom position**.
Similarity * (Similarity Search)	・**Substances that are similar to the queried structure** in addition to the substances retrieved by Exact Search – Substances containing different elements or element's positions than the queried structure – Substances that do not match the queried structure exactly (e.g.: For ethyl group, methyl group can be retrieved) – Substances containing different cyclic structure than the queried structure (e.g.: For 6–5 membered ring, 6–6 membered ring can be retrieved)

＊ Similarity score is calculated based on a Tanimoto metric.

■ Relation between three search types

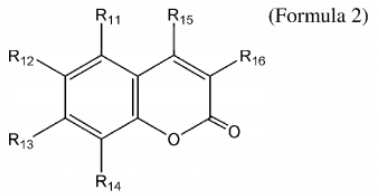


For the details, see www.jaici.or.jp/scifinder-n/ref/sfn_strtype.pdf.

Tips: Markush structure search (MARPAT)

■ Use a Patent Markush search to find patents that have generic formula (Markush structure) described in the claims matching your query.

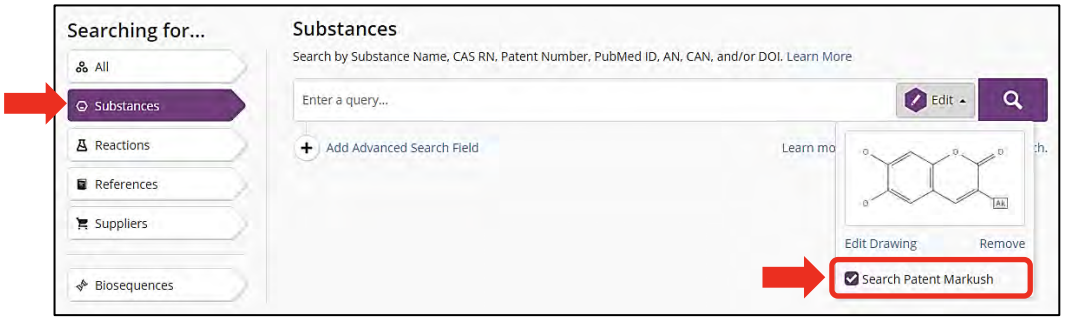
e.g.: WO2014204104



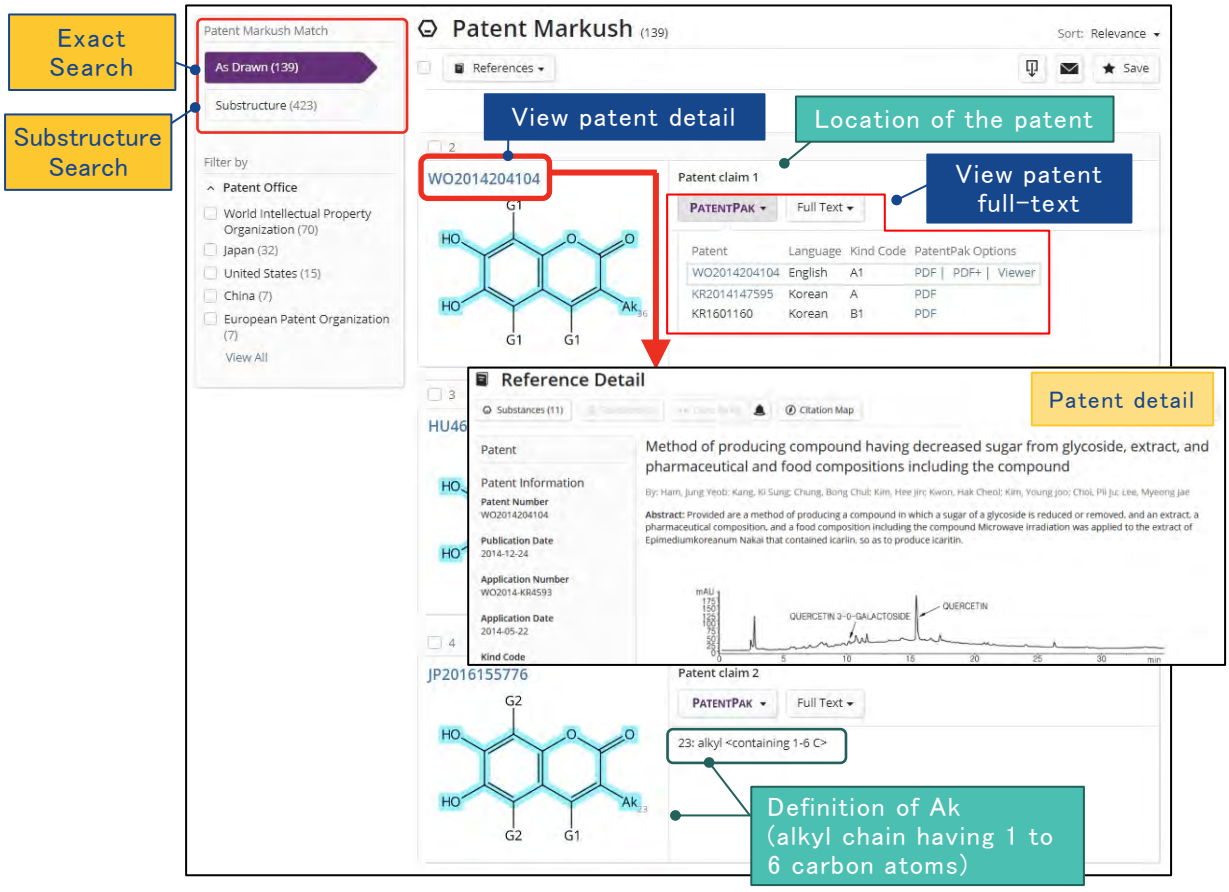
(Formula 2)

in Formula 2, R11, R12, R13, R14, R15, and R16 are each independently -H, -OH, -OR19, or -R20, and wherein R19 and R20 are each independently C1-C20 alkyl, C2-C20 alkenyl, or C2-C20 alkynyl and at least one of R11, R12, R13, R14, R15, and R16 is hydroxyl group.

■ To find patents by a Patent Markush search, check the box for Search Patent Markush.



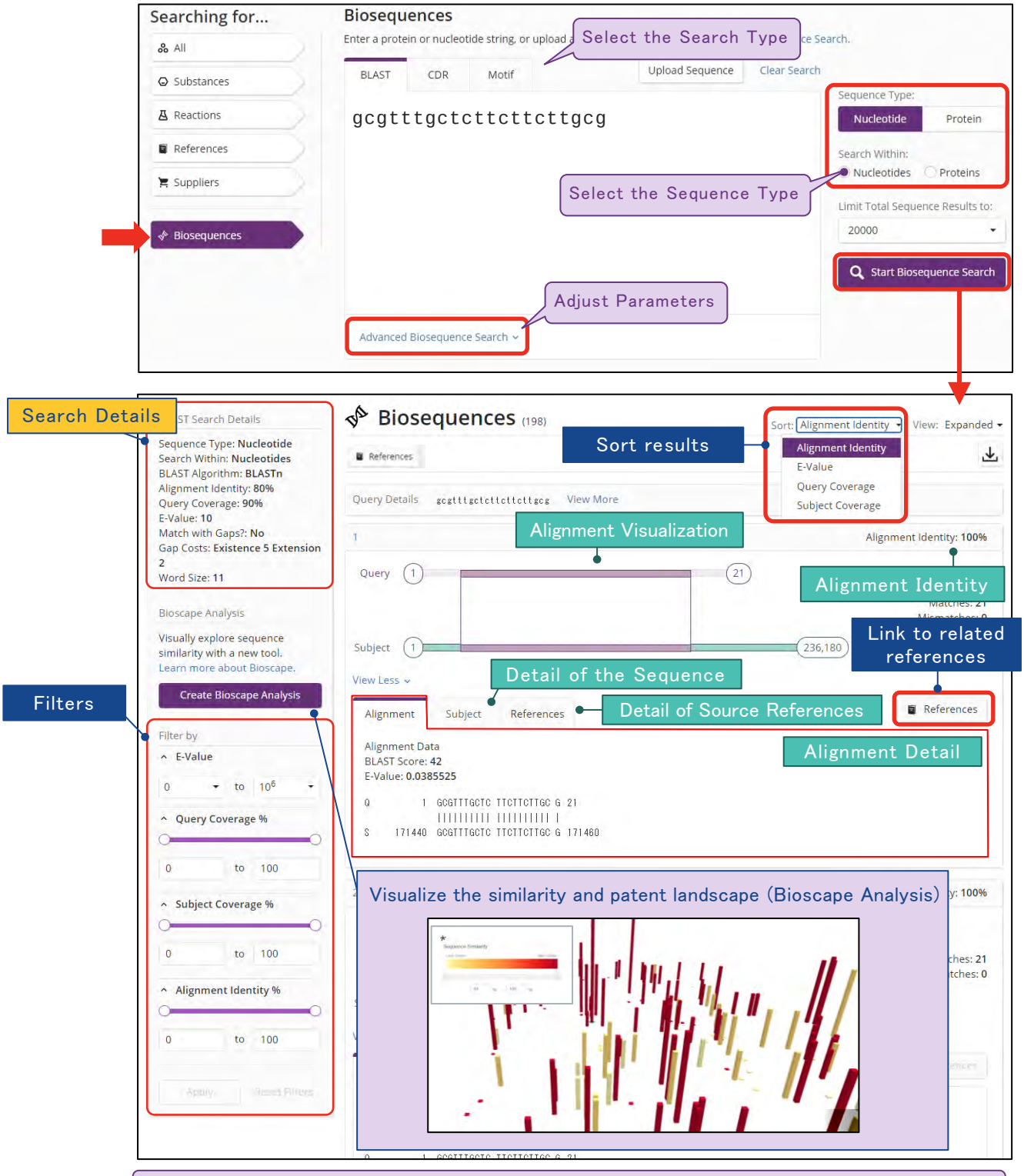
・ If multiple Markush structures in the patent match your query, all those structures are retrieved.



Tips: Biosequence search

■ In the Biosequene search, there are following three search types.

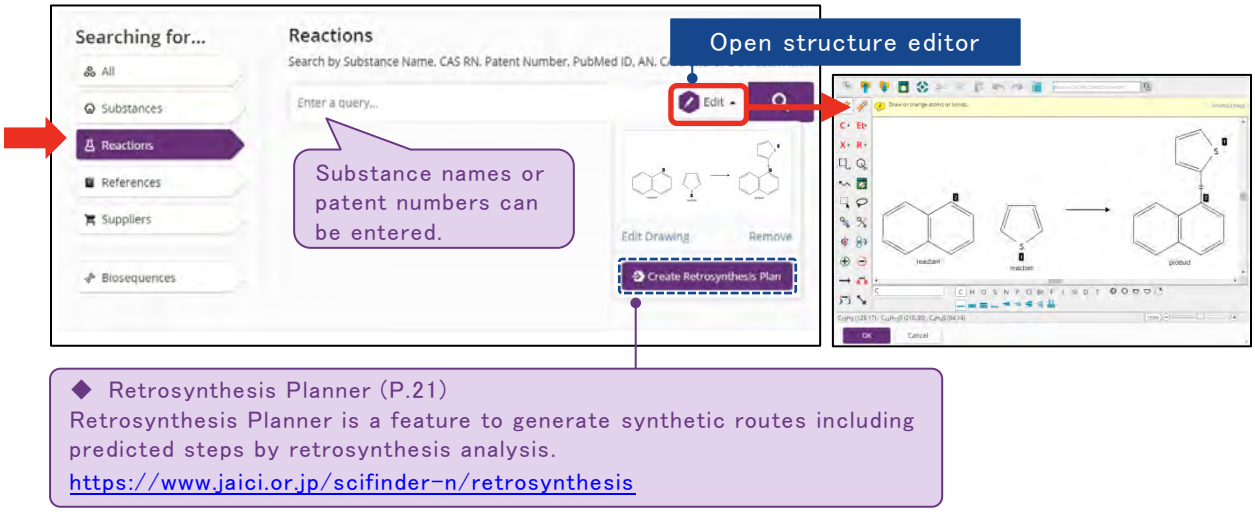
- BLAST: Search for proteins as well as nucleotides using a set of local alignment algorithms.
- CDR: Search for antibody and t-cell receptors.
- Motif: Search for short patterns in DNA, RNA, or proteins



For the details of Biosequences Search, Bioscape Analysis or search for nucleic acid or protein/peptide, see www.jaici.or.jp/scifinder-n/ref/sfn_bioseq.pdf.

Reaction search

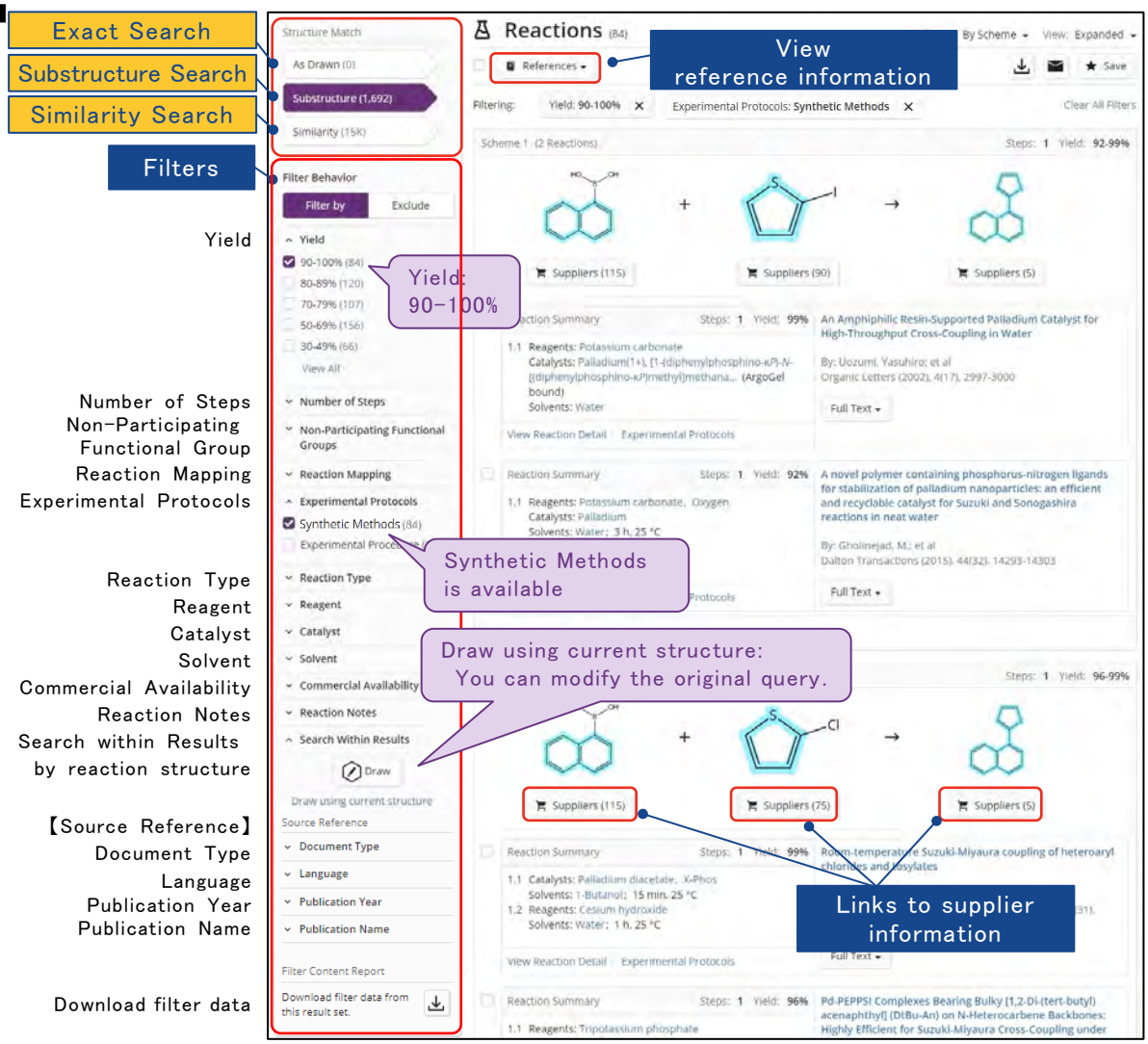
■ In the Reaction search, you can find reactions by substance name, chemical structure, CAS Registry Number (CAS RN®), etc.



◆ Retrosynthesis Planner (P.21)
Retrosynthesis Planner is a feature to generate synthetic routes including predicted steps by retrosynthesis analysis.
https://www.jaici.or.jp/scifinder-n/retrosynthesis

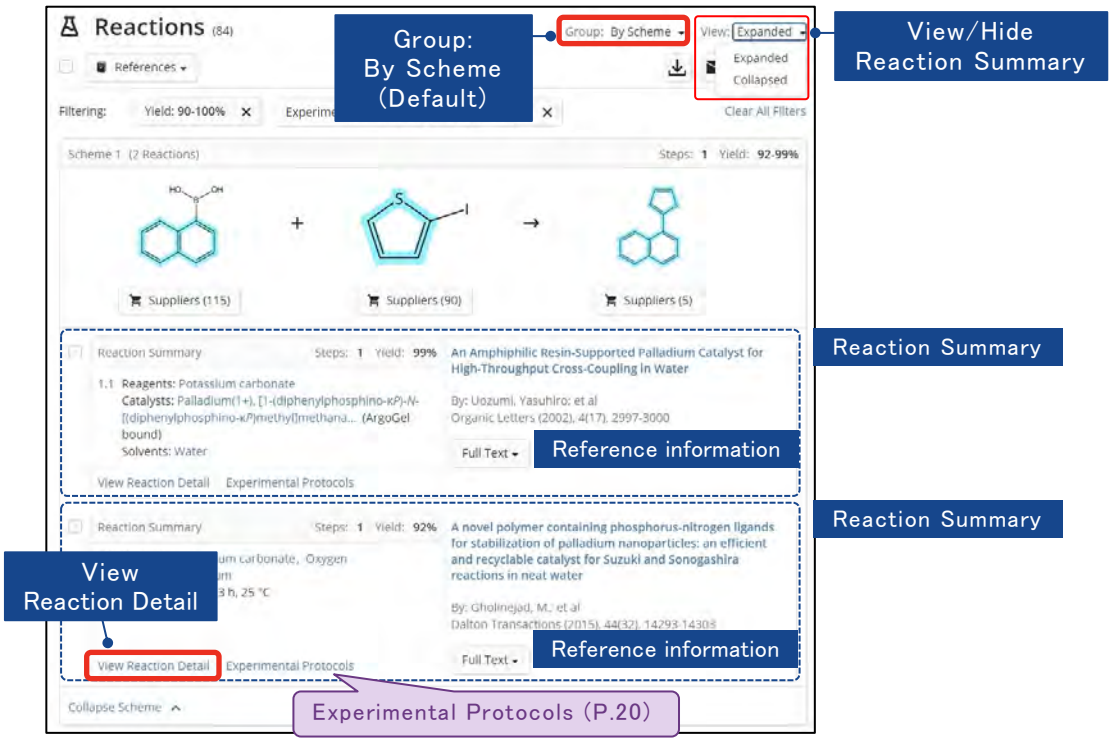
■ Select the type you wish to view from Structure Match. To focus the result set, select filters from Filter by or Exclude on the left side of the page.

■

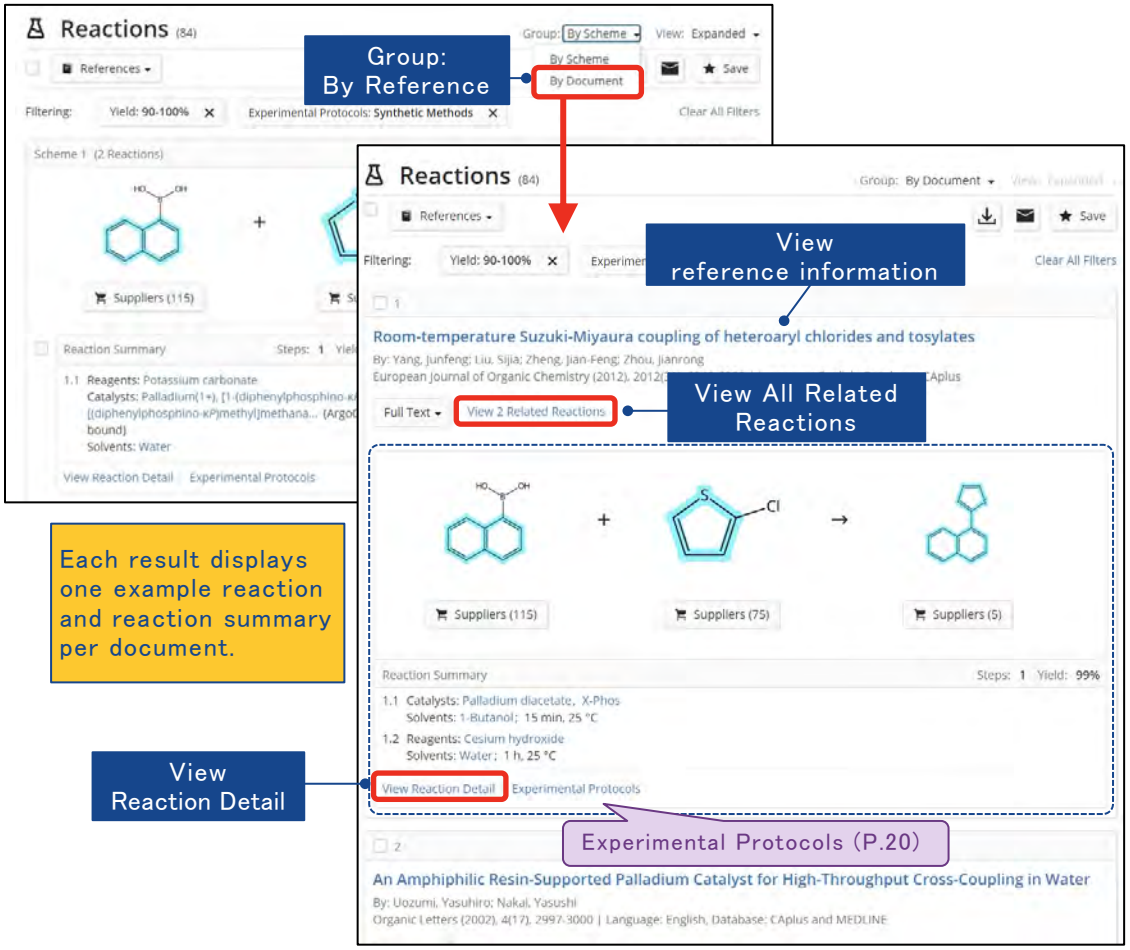


- Results are grouped by scheme (default)

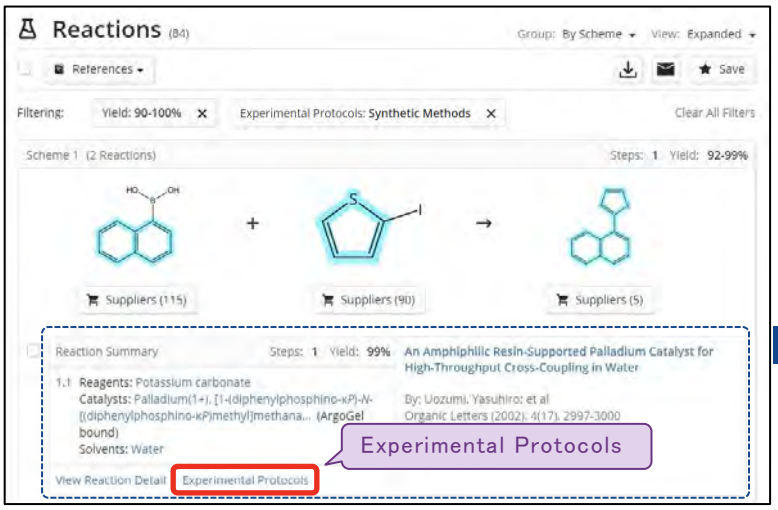
  - Each scheme contains reactions that have the same reactants and products.



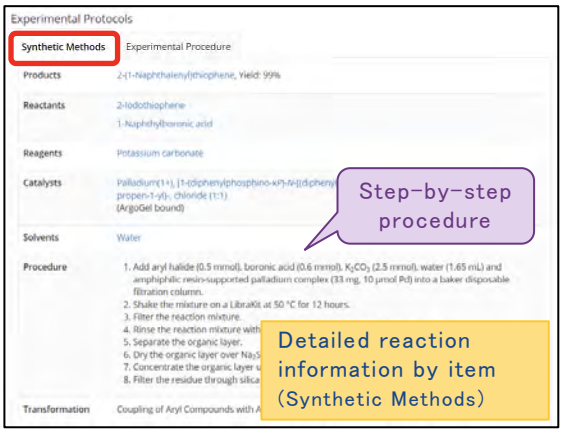
  - By Document groups reactions by the document in which they are referenced.



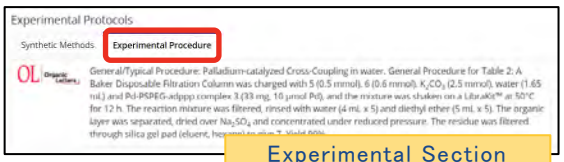
- To view a reaction detail, click Experimental Protocols.



Synthetic Methods



Experimental Procedure



– Contents of Experimental Protocols

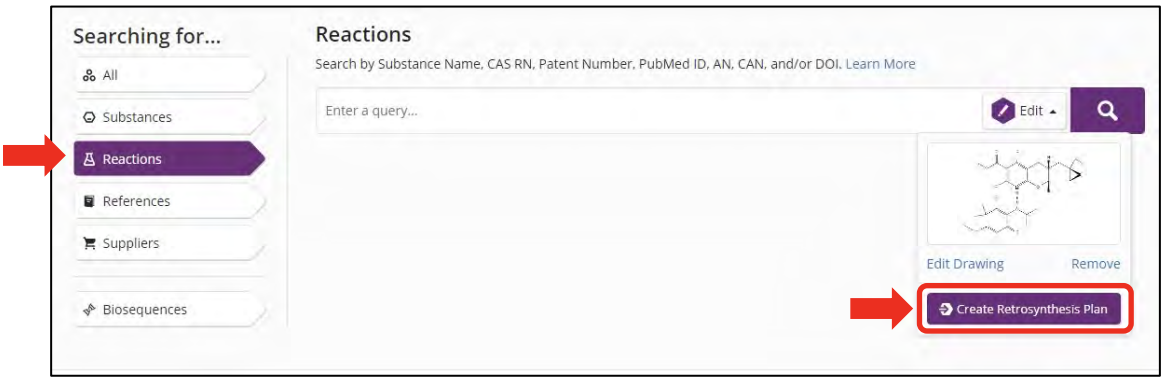
Synthetic Methods	
Journals	2000–
ACS	: Journal of Medicinal Chemistry, Journal of the American Chemical Society
Springer	: Catalysis Letters
Taylor & Francis	: Journal of Coordination Chemistry
Elsevier	: Tetrahedron
RSC	: Chemical Science
Wiley	: Angewandte Chemie etc, (about 180 journals)
WIPO patents (English)	2010–
Experimental Procedure	
Journals	Mainly 1998–
ACS	: All journals
Taylor & Francis	: Synthetic Communications, Journal of Coordination Chemistry, etc
Springer	: 165 journals in Chemistry (1985–)
Shanghai institute of Organic Chemistry	: Youji Huaxue, Huaxue Xuebao
Thieme	: SYNLETT (1989–2013), SYNTHESIS (1980–2013)
SORD	: Selected Organic Reactions Database (dissertations,1961–2011)
Patents	2000–
English	: US (America), EP (Europe), WIPO (World Intellectual Property Organization), CA (Canada), GB (Great Britain)
Japanese	: JP (Japan), WIPO (World Intellectual Property Organization)
German	: DE (Germany), EP (Europe), WIPO (World Intellectual Property Organization)

Tips: **Retrosynthesis Planner**

■ Retrosynthesis Planner creates viable synthetic steps to the target substance based on known reactions in CASREACT (For more detail, see www.jaici.or.jp/scifinder-n/ref/sfn_retrosynthesis.pdf).

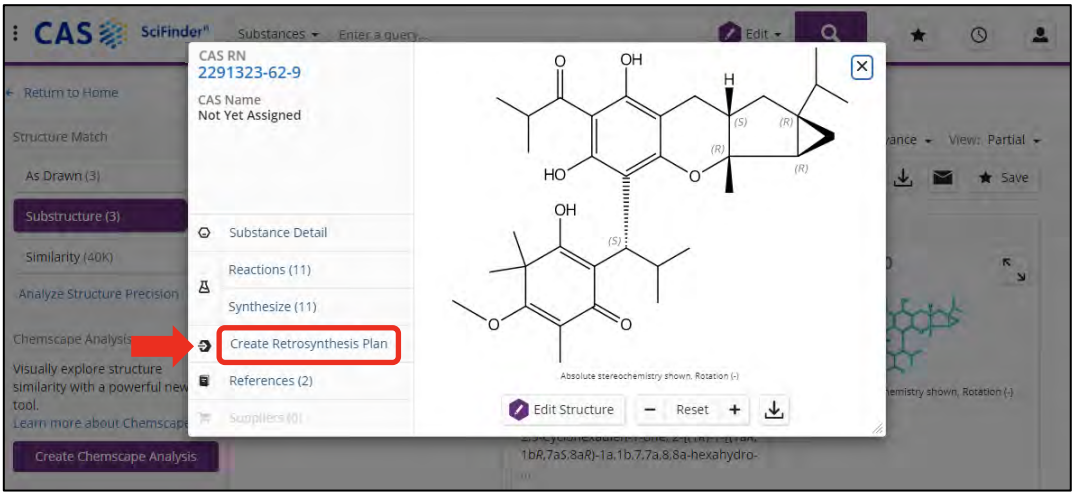
- From the Reactions Search page

  - Draw a structure on the Reactions page, and then click the Create Retrosynthesis Plan button displayed under the structure image.



- From a substance window

  - After opening the substance window by clicking a substance structure image, Click the Create Retrosynthesis Planner button on the left side of the substance window.

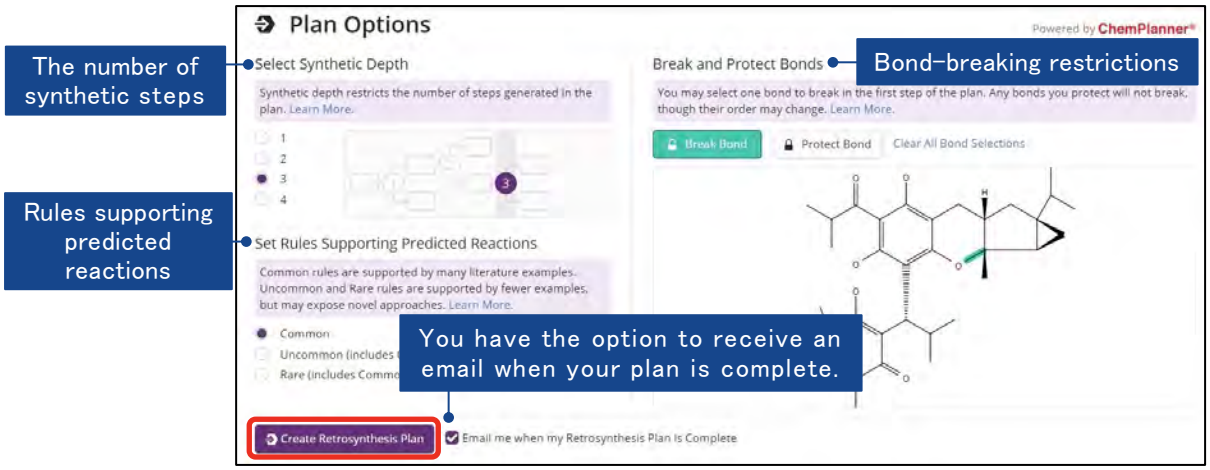


- You can continue to work within CAS SciFinder^{n} while waiting for your Retrosynthesis plan to complete.

Open created Retrosynthesis Plan

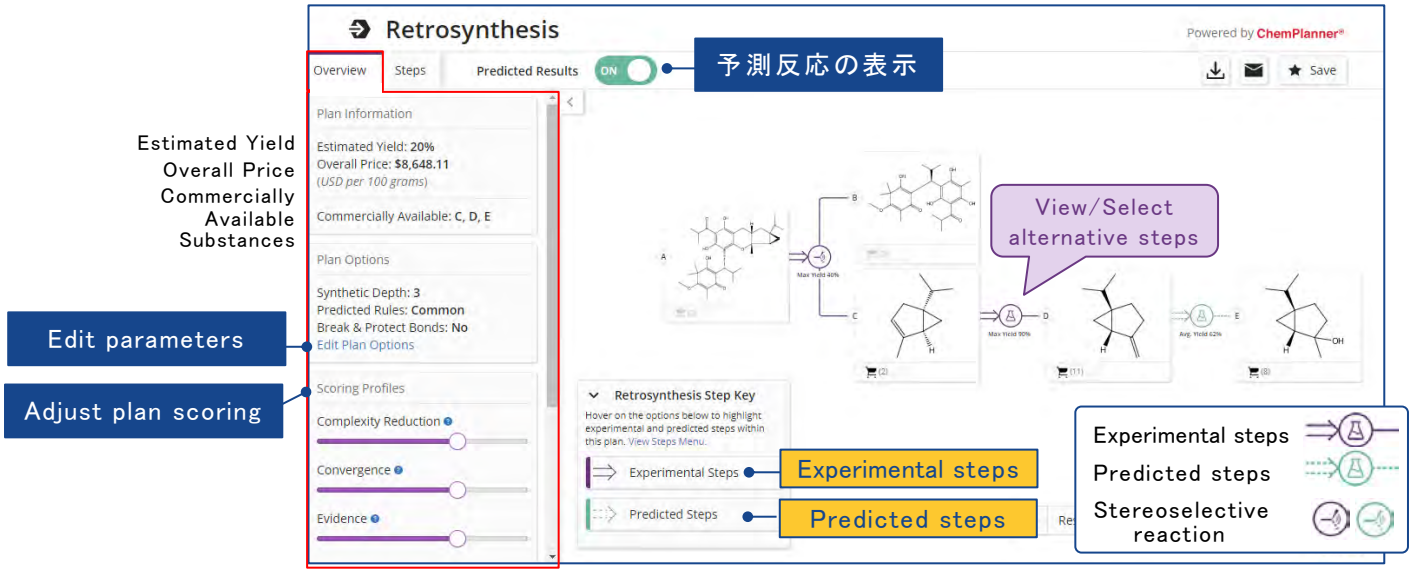
You can open created Retrosynthesis plan from the ★ (Save) button or the 🕒 (History) button. Saved retrosynthesis plans expire 90 days after the date they are first generated.

■ Plan Options page appears after clicking the Create Retrosynthesis Plan button.



- To apply your edits to the options and generate your plan, click the Create Retrosynthesis Plan button.

■ Overview and Steps tabs are displayed in Retrosynthesis Plan page. Red lines are experimental steps and green ones are predicted steps.



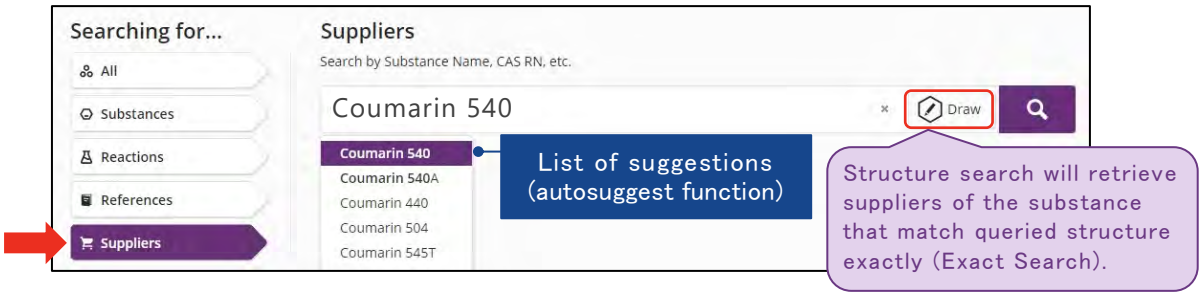
- The Overview tab has estimated yield, overall cost, and commercially available substances in the current retrosynthesis plan.
  In the Scoring Profiles, you can set scoring profiles that determine what is displayed in the plan/alternative steps.

- The Steps tab provides the summary of all steps in the current retrosynthesis plan.

  - Evidence : View reactions and references supporting the plan step.
  - Alternative Steps : View and select alternatives for a plan step.

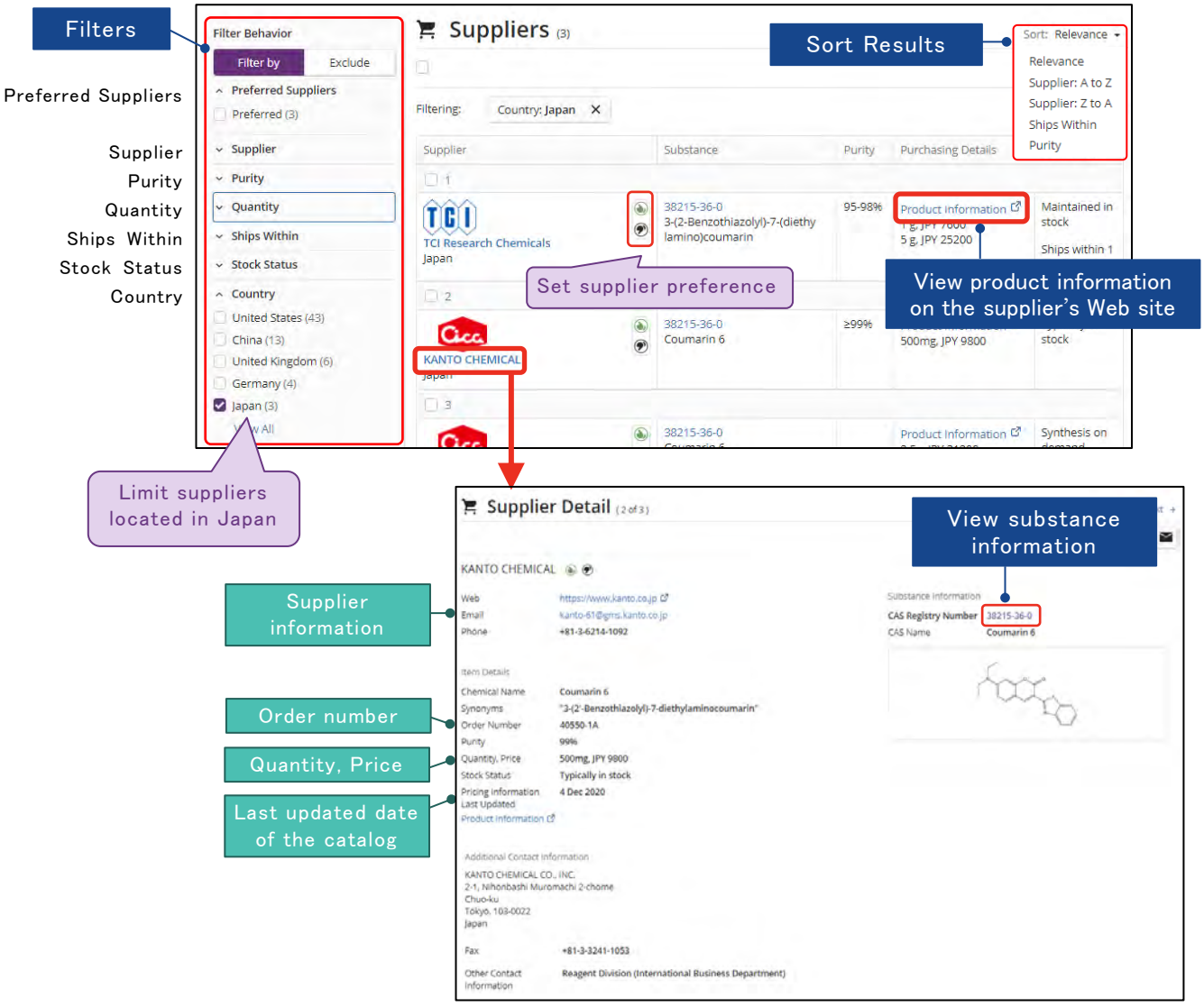
Supplier search

■ In the Supplier search, you can find suppliers by substance name, chemical structure, etc.



■ Answers are sorted by Relevance by default.

- Click to specify a supplier as Preferred. Preferred suppliers will appear at the top of the list.
- Select filers to display or exclude answers that match the applied filters.
- To view its supplier detail page, click the supplier name.

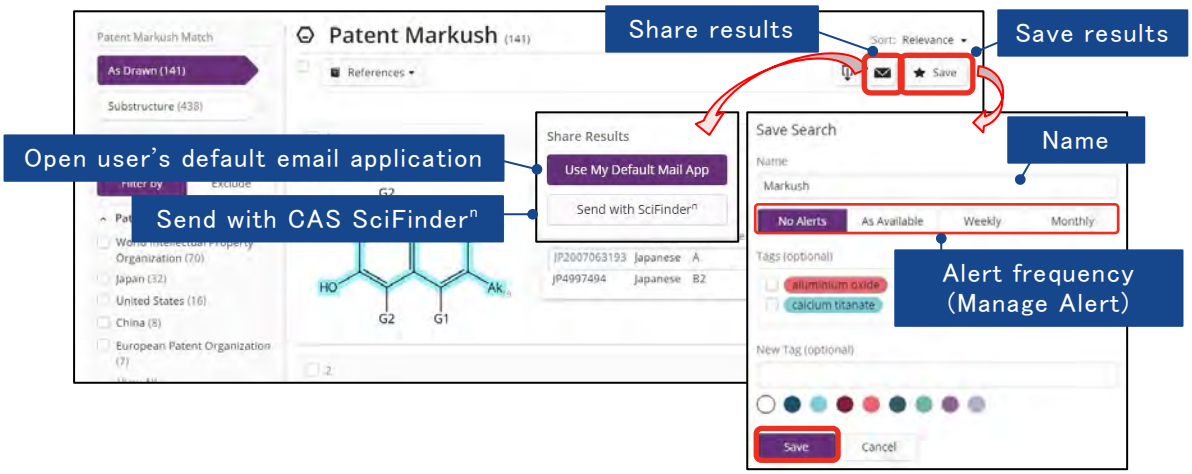


Saving, Alerts, and Sharing

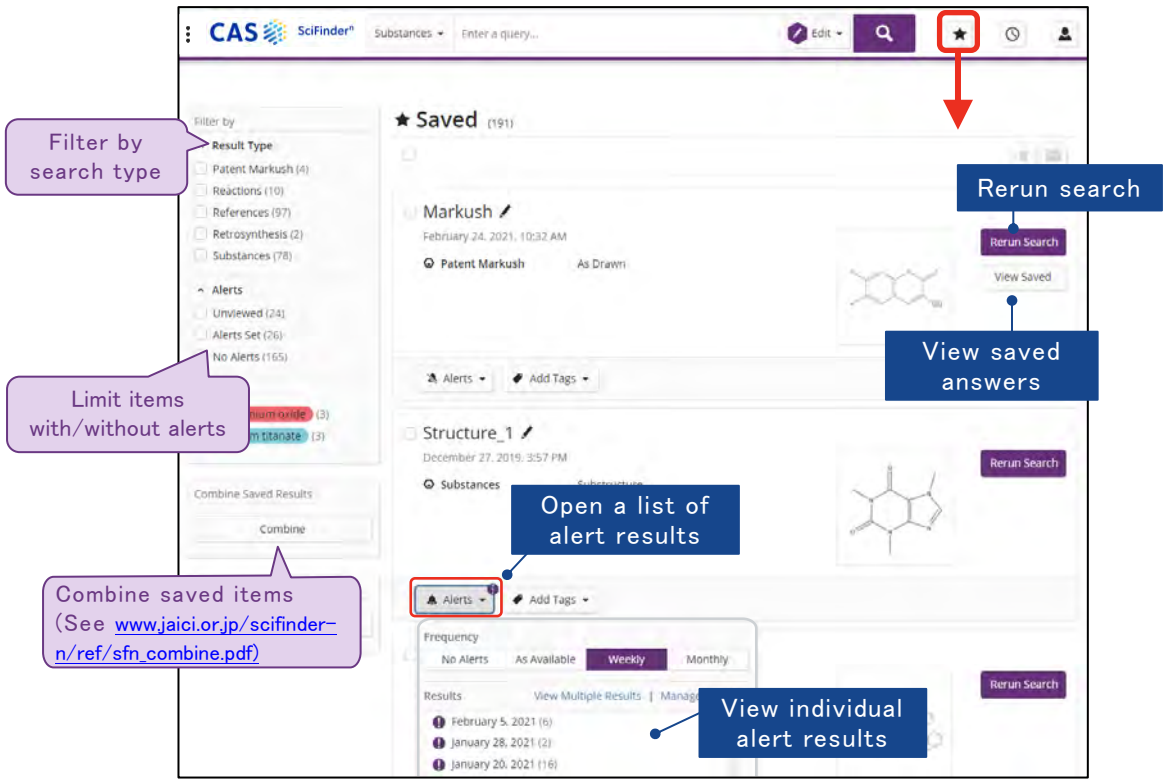
■ Selected results and the search can be saved or shared with other users.

- Click the Email icon to share results with a colleague via email.
  - You can share your results including keywords and/or structures with filter items you used.
  - You can share your results within the same organization.

- Click the Save button to save text/structure query including applied filter items.
  - To save individual answers, select check boxes of individual results you wish to save, and then click the Save button.
  - To set an alert, click the Save button then select a frequency from As Available (new content added), Weekly, or Monthly.

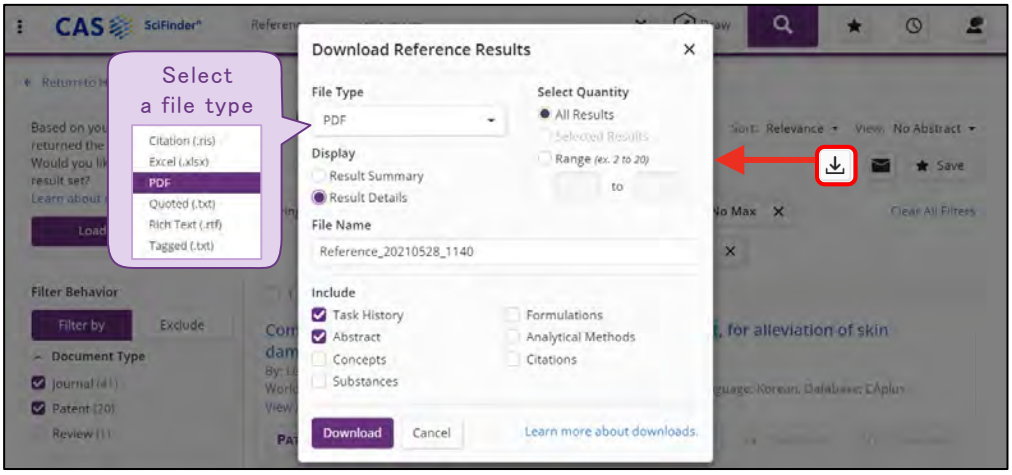


  - To access the saved searches and results, click ★ button on the top menu bar.



Download results

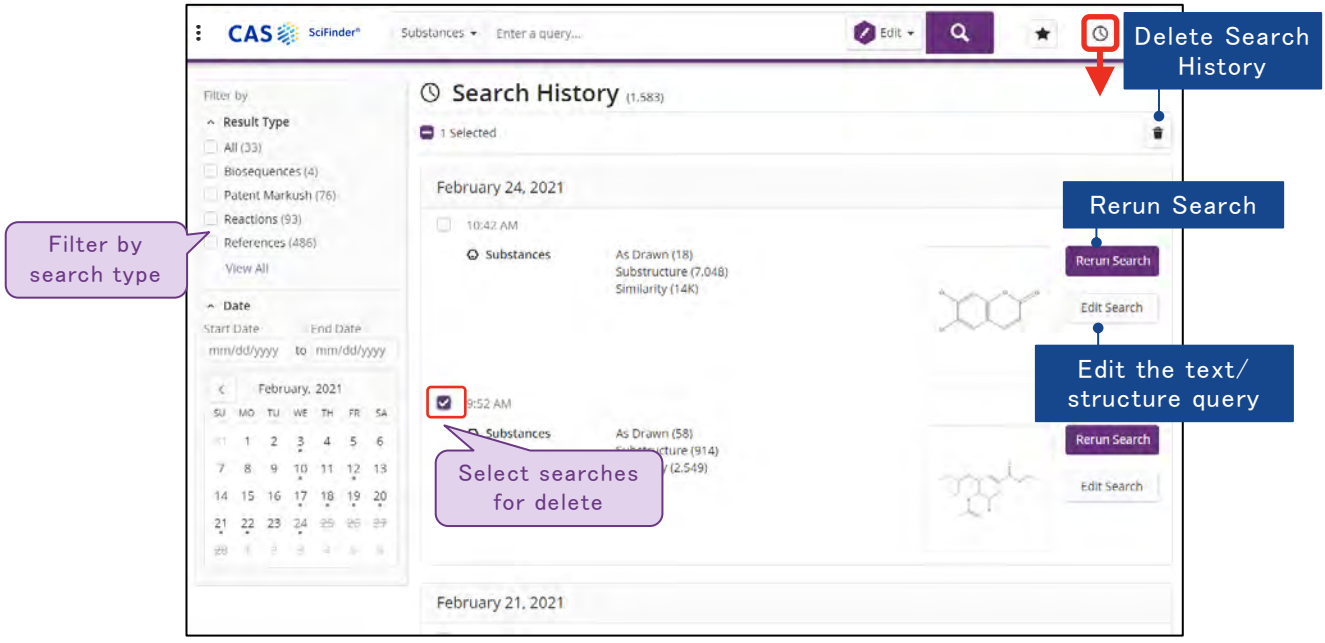
■ CAS SciFinderⁿ supports multiple data formats for downloading results.



- You can share your downloaded answers within the same research group.
- Up to 500 or 100 answers can be downloaded at one time
- Users are not allowed to keep more than 5,000 downloaded answers at any given time under the license agreement. Answers exceeding 5,000 shall be deleted.

Search history

■ To access the search history page, click the clock icon at the top of any page.



- Text/structure queries you used before clicking the icon are recorded on the Search History page. Filters used after the search are not included.

Tips: Contents of CAS SciFinder^n

■ Main contents of CAS SciFinder^n

- References published in more 50 languages that are searchable in English
- Journal
  - Journals in science and technology fields (several thousands)*
    * Bibliographic information of major 1,500 journals is added within 1 week of journal receipt in CAS
  - Journals in biology and medical fields (several thousands)
- Patents
  - Patents in Chemical and surrounding area around the world (several thousands)*
    * Bibliographic information of patents from major countries is added within 2 days of the patent's issuance and fully indexed by CAS scientists in less than 27 days from the date of issue.

■ Area of contents (CAS References)

Biochemistry	36%
Applied Chemistry	25%
Physical, Inorganic, Analytic Chemistry	24%
Polymer Chemistry	9%
Organic Chemistry	6%

■ Substance Type

- Organic Compounds
- Inorganic Compounds
- Nucleic acids, Proteins
- Coordination Compounds
- Polymers
- Alloys

■ Searchable information in CAS SciFinder^n

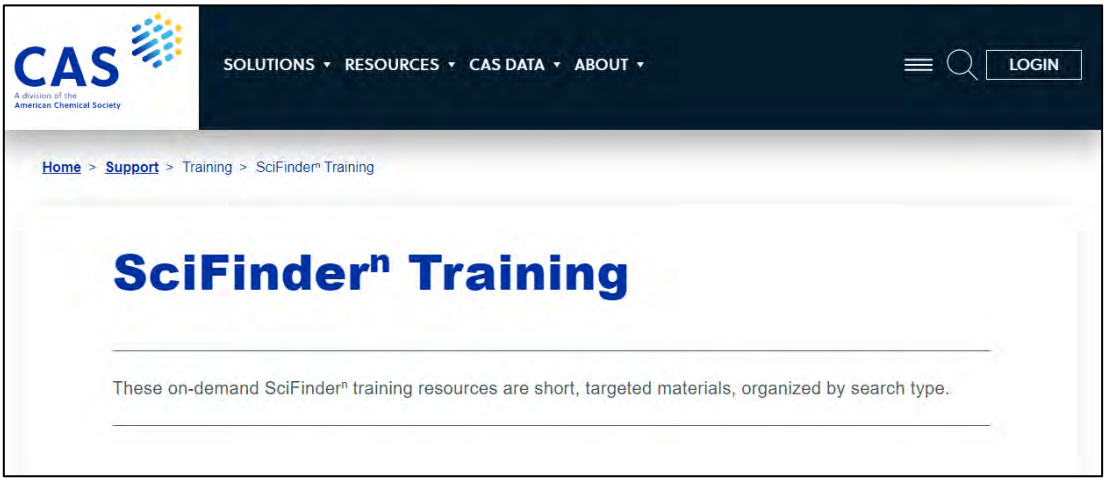
(As of July 2021)

Category	Contents	Amount of information	Year
Reference	Chemistry and surrounding area【CAS References】	> 54 million references	1808–
	Biology and medical area 【MEDLINE】	> 32 million References	1946–
	Patents with Markush structure【CAS Markush】	> 54 thousand References (patent) > 1.9 million Markush structures	1961–
	Chemistry area in old era (option)【CAS ChemZent】	> 3 million References	1830 – 1969
Substance	Chemical name, CAS Registry Number (CAS RN®), molecular formula, chemical structure, sequence, physical property, etc. 【CAS REGISTRY】	> 2.47 million Substances	Early 1800–
Reaction	Organic chemical reactions 【CAS Reactions】	> 1.18 million Reactions > 1.9 million References	1840–
Catalog	Catalog information 【Commercial Sources】	Hundreds of Catalog information provided by chemical vendors around the world	As available
Regulatory	Inventory and regulatory information around the world	> 400 thousand Substances	1979–

Training materials

■ JAICI offers Japanese training materials on https://www.jaici.or.jp/scifinder-n/doc.html .
We also offer links to English training materials created by CAS.

・ You can use another English training and on-demand materials on CAS Web site.
(https://www.cas.org/support/training/scifinder-n)



Helpdesk (9 a.m. – 5 p.m. weekdays, Japan standard time)

Users in Japan can contact us if you have questions or need information about CAS SciFinder^n.

e-mail support@jaici.or.jp

* For users outside of Japan, please contact help@cas.org for support.

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