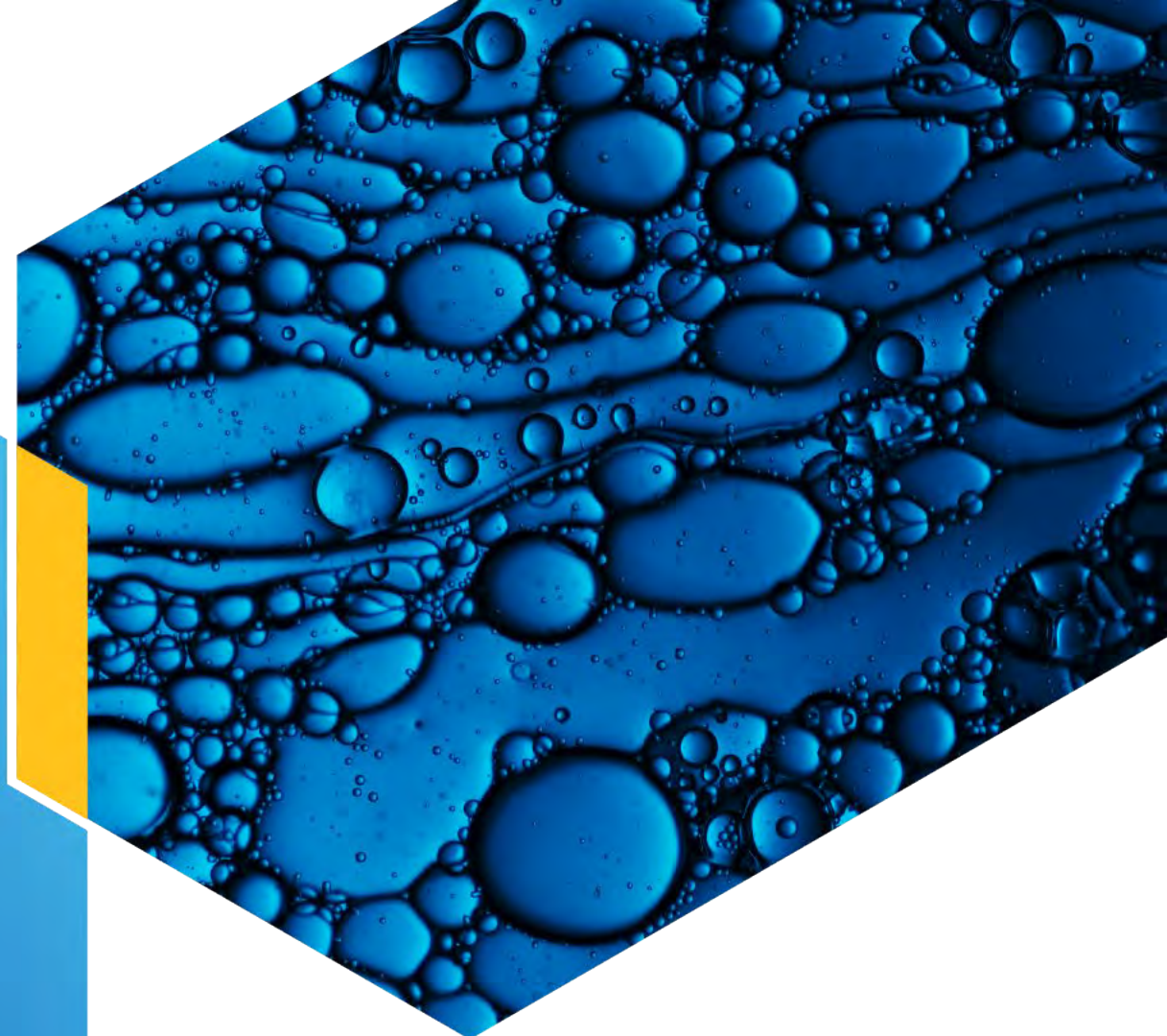


STNext

Analyzing the chemical space more efficiently with Chemscape



Agenda

Analyzing the chemical space more efficiently with Chemscape

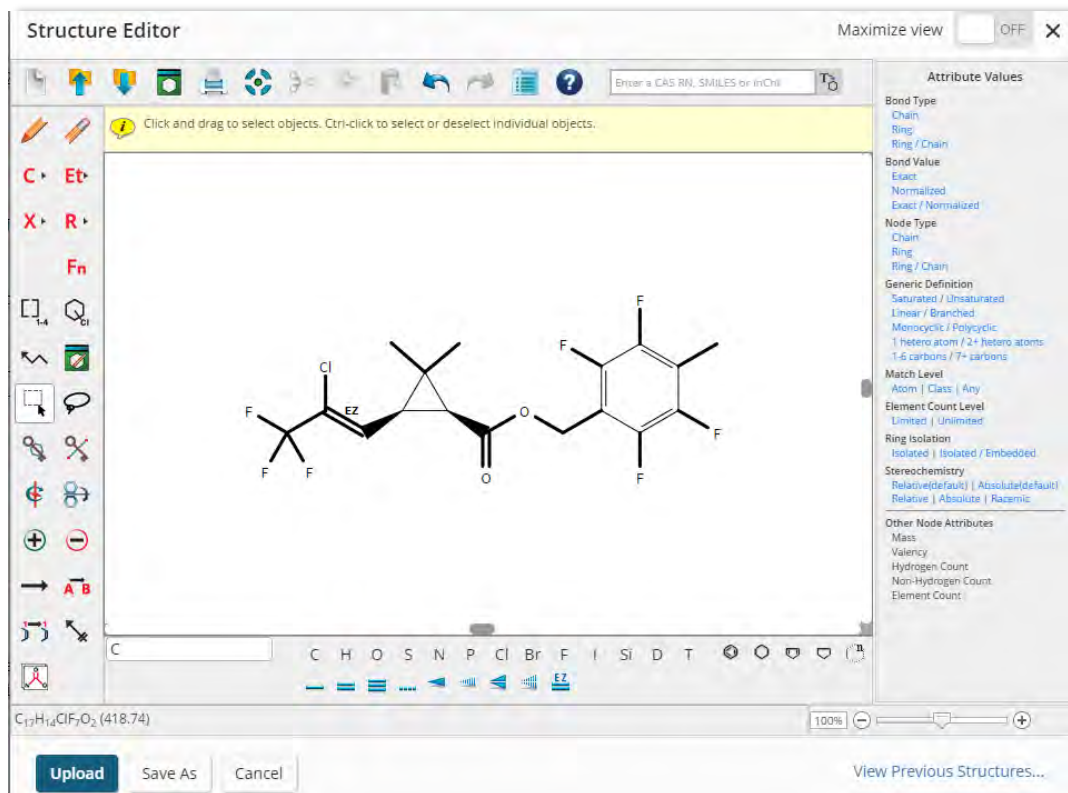
- What is Chemscape?
- How to create Chemscape Analyses
- Use cases

What is Chemscape?

- Chemscape visualizes the similarity and patent landscape for a set of substance results
- Location of substance bar corresponds to the similarity of the query structure – initial structure search is required for Chemscape analyses!
- Height of substance bar corresponds to the number of patents in which the substance has been indexed
- Chemscape offers different types of graphical analyses

How to create Chemscape analyses

- In order to provide the graphical overview based on similarity, STNext needs a structure query



L2 STRUCTURE UPLOADED

=> s 12 fam full

FULL SEARCH INITIATED 03:45:33

FULL SCREEN SEARCH COMPLETED - 414 TO ITERATE

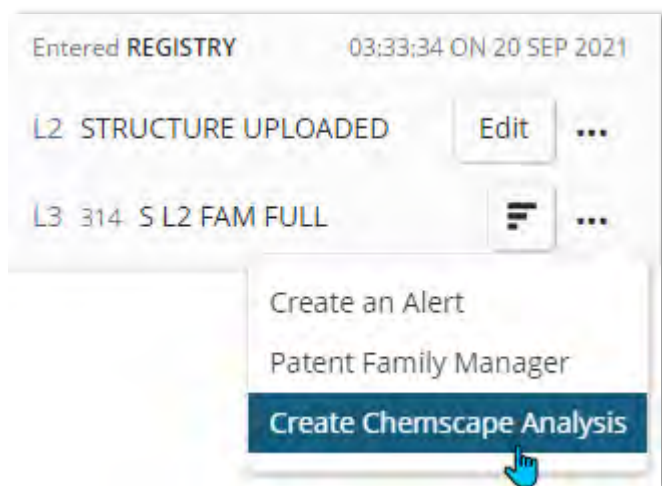
100.0% PROCESSED 414 ITERATIONS

SEARCH TIME: 00.00.01

314 ANSWERS

How to create Chemscape analyses

- In your history tab you will be able to select „Create Chemscape Analysis“ via the ellipsis
- Select the answers you like to include – up to 1000 are possible
- Chemscape analysis will be created, initially colored by structural similarity



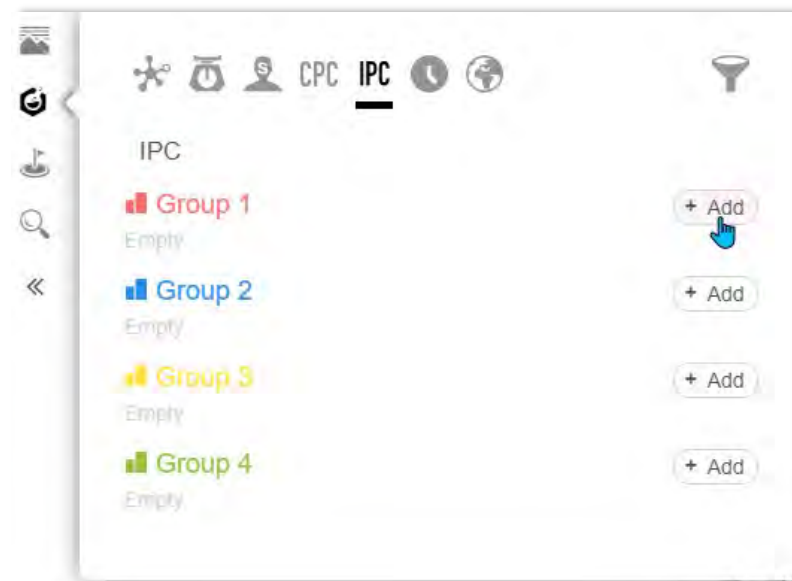
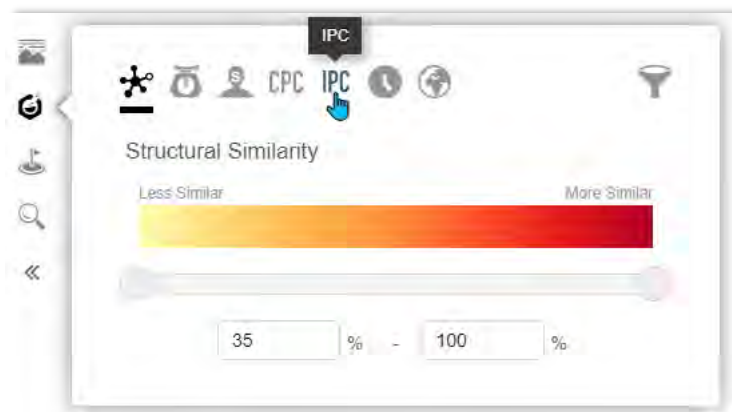
STNext - Chemscape Use Cases



Chemscape – Use Cases

Analysis by applications

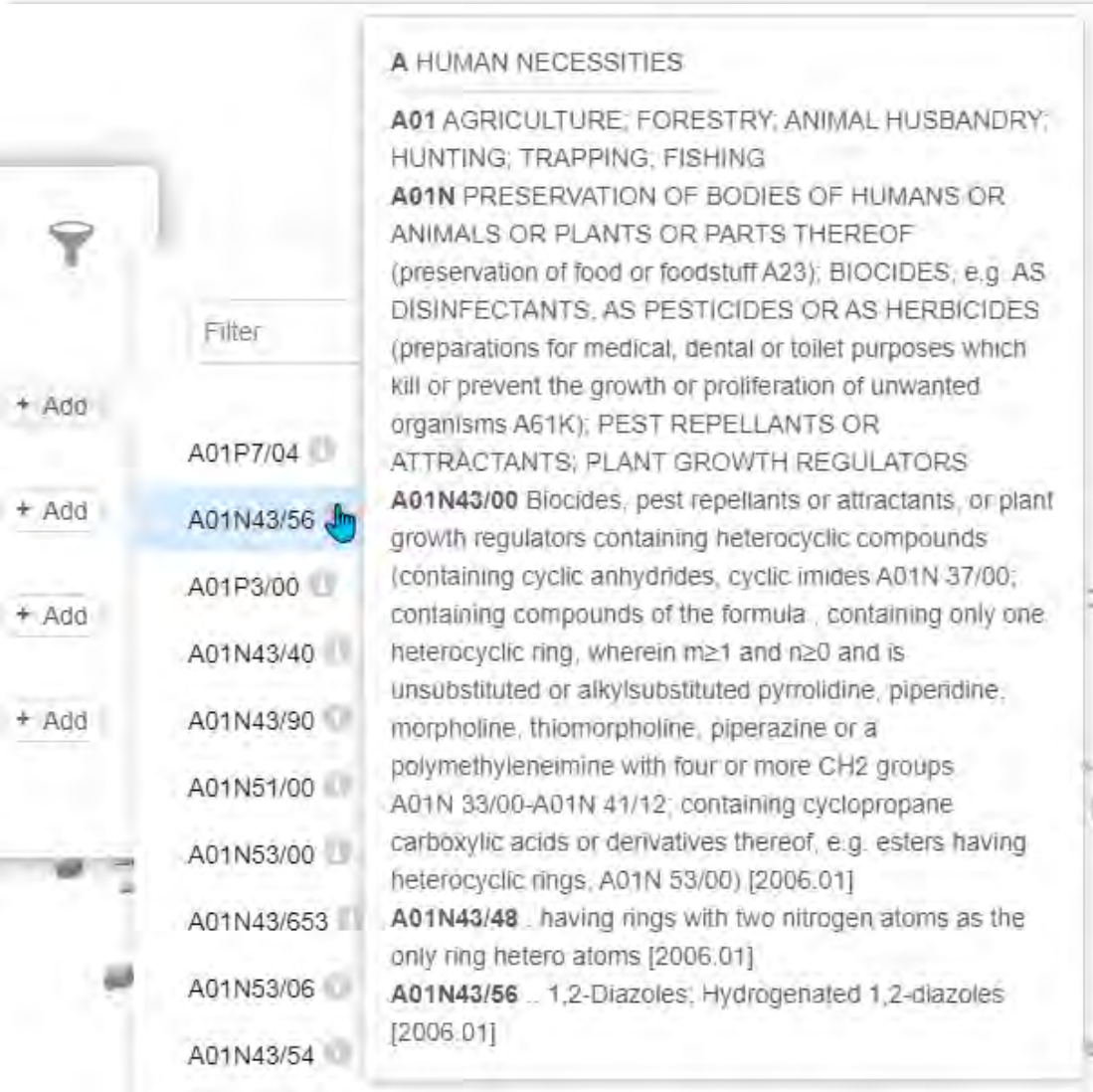
- You can analyze the landscape based on CPC and IPC codes
- Color your landscape by up to 4 different groups of classification codes



Chemscape – Use Cases

Analysis by applications

- Hover over the  to learn more about the meaning of the classification code



The screenshot shows a sidebar with a list of classification codes and a main panel displaying a detailed tooltip for the selected code, A01N43/56. The tooltip is titled "A HUMAN NECESSITIES" and provides a comprehensive description of the code's scope and sub-classifications.

A HUMAN NECESSITIES

A01 AGRICULTURE; FORESTRY; ANIMAL HUSBANDRY; HUNTING; TRAPPING; FISHING

A01N PRESERVATION OF BODIES OF HUMANS OR ANIMALS OR PLANTS OR PARTS THEREOF (preservation of food or foodstuff A23); BIOCIDES, e.g. AS DISINFECTANTS, AS PESTICIDES OR AS HERBICIDES (preparations for medical, dental or toilet purposes which kill or prevent the growth or proliferation of unwanted organisms A61K); PEST REPELLANTS OR ATTRACTANTS; PLANT GROWTH REGULATORS

A01N43/00 Biocides, pest repellants or attractants, or plant growth regulators containing heterocyclic compounds (containing cyclic anhydrides, cyclic imides A01N 37/00; containing compounds of the formula C_nH_mN , containing only one heterocyclic ring, wherein $m \geq 1$ and $n \geq 0$ and is unsubstituted or alkylsubstituted pyrrolidine, piperidine, morpholine, thiomorpholine, piperazine or a polymethyleneimine with four or more CH_2 groups A01N 33/00-A01N 41/12; containing cyclopropane carboxylic acids or derivatives thereof, e.g. esters having heterocyclic rings, A01N 53/00) [2006.01]






A01N43/48 ... having rings with two nitrogen atoms as the only ring hetero atoms [2006.01]

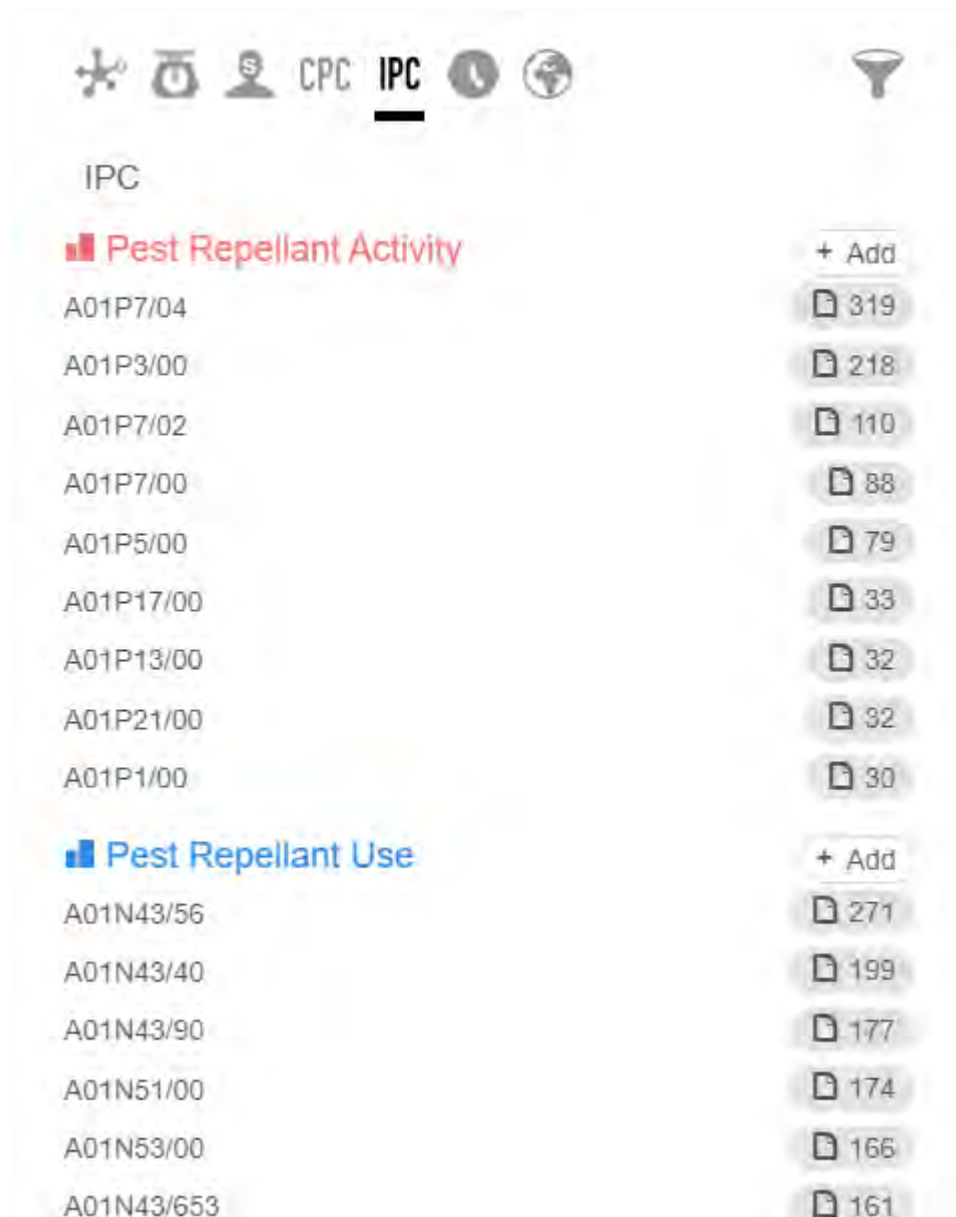
A01N43/56 ... 1,2-Diazoles; Hydrogenated 1,2-diazoles [2006.01]

Chemscape – Use Cases

Analysis by applications

- After selecting multiple classification codes, you can rename the group, so that the legend will be adapted

 Pest Repellant Activity	163
 Pest Repellant Use	299
 Seed Treatment	16
 Mixtures	2
 Other structures	1



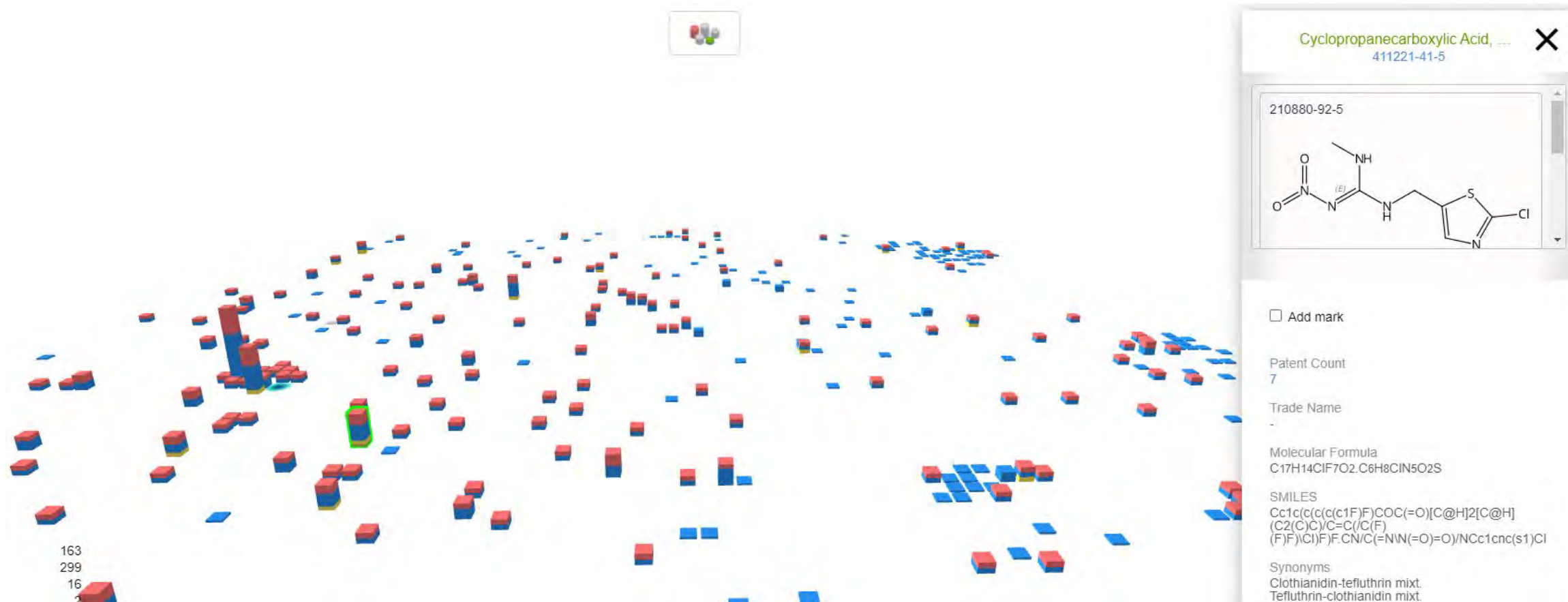
The screenshot shows the Chemscape interface with the 'IPC' classification selected. The interface displays a list of classification codes and their corresponding counts. The 'Pest Repellant Activity' group is highlighted in red, and the 'Pest Repellant Use' group is highlighted in blue. Each code has a '+ Add' button and a count button.

Classification Code	Count
IPC	
Pest Repellant Activity	+ Add
A01P7/04	319
A01P3/00	218
A01P7/02	110
A01P7/00	88
A01P5/00	79
A01P17/00	33
A01P13/00	32
A01P21/00	32
A01P1/00	30
Pest Repellant Use	+ Add
A01N43/56	271
A01N43/40	199
A01N43/90	177
A01N51/00	174
A01N53/00	166
A01N43/653	161

Chemscape – Use Cases

Analysis by applications

- Click on a bar shows you structure and option to get to patents with selected analysis



Chemscape – Use Cases

Analysis by applications

Get Patents from STN File

STN File

<input type="radio"/> AUPATFULL	<input type="radio"/> GBFULL	<input type="radio"/> PCTFULL
<input type="radio"/> CANPATFULL	<input type="radio"/> HCAPLUS	<input type="radio"/> PCTGEN
<input checked="" type="radio"/> CAPLUS	<input type="radio"/> IFIALL	<input type="radio"/> USGENE
<input type="radio"/> CNFULL	<input type="radio"/> INFULL	<input type="radio"/> USPATFULL
<input type="radio"/> DEFULL	<input type="radio"/> INPADOCDB	<input type="radio"/> WPIINDEX
<input type="radio"/> DGENE	<input type="radio"/> INPAFAMDB	<input type="radio"/> WPIX
<input type="radio"/> EPFULL	<input type="radio"/> JPFULL	<input type="radio"/> ZCAPLUS
<input type="radio"/> FRFULL	<input type="radio"/> KRFULL	

Save Script

Each request is limited to 5000 patents.

Continue Cancel

L5 7 (CN102696659A OR JP2008133240A OR CN102763681A OR WO2002-030202A2 OR WO2008-092819A2 OR CN102379308A OR US20140020611A1)/PN

=> d bib abs ind hitppak

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2021 ACS on STN
[PatentPak PDF](#) | [PatentPak PDF+](#) | [PatentPak Interactive](#)

AN 2014:105691 CAPLUS Full-text

DN 160:242870

TI Method for reducing damage by harmful organisms in corn cultivation using pesticide combinations

IN Sakamoto, Norihisa; Ozawa, Mayuko; Iwata, Atsushi

PA Sumitomo Chemical Company, Limited, Japan

SO U.S. Pat. Appl. Publ., 12pp.

CODEN: USXXCO

DT Patent

LA English

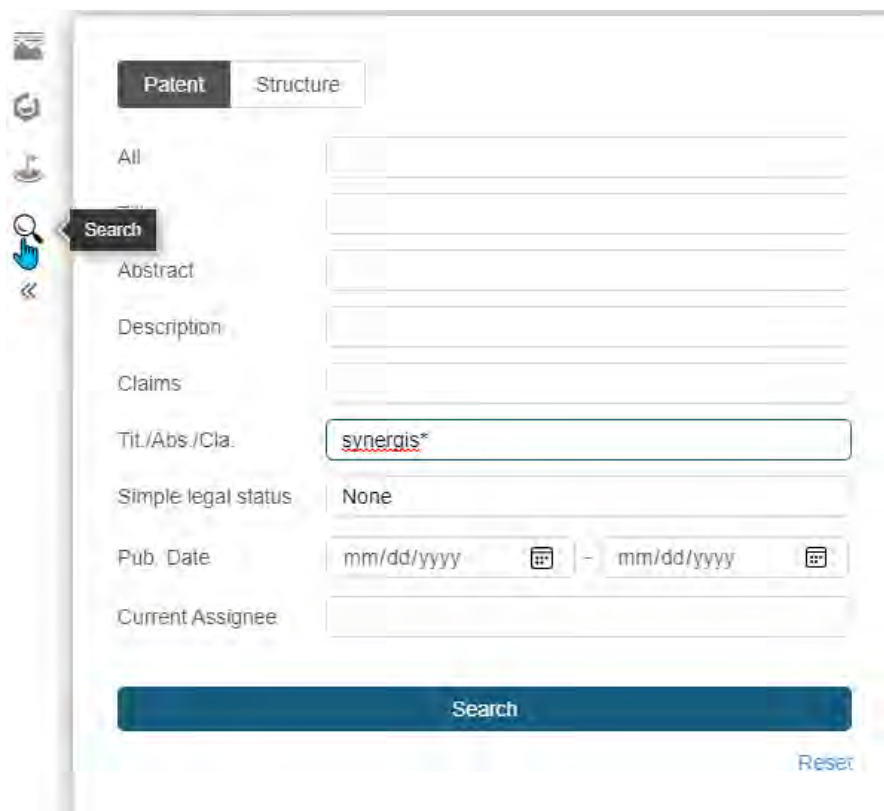
FAN.CNT 1

PPPI

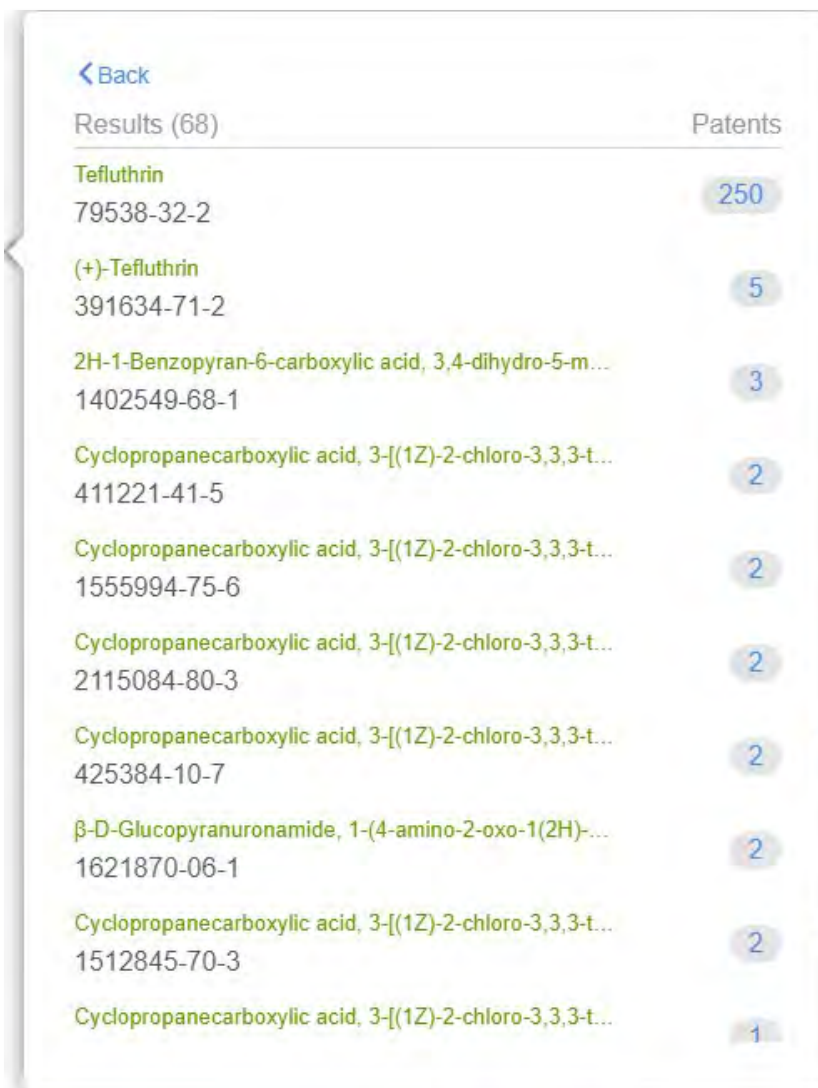
PATENT NO.	KIND	DATE	LANGUAGE	PatentPak
US 20140020611	A1	20140123	English	PDF PDF+ Interactive
US 9439415	B2	20160913	English	PDF
ES 2439615	A2	20140123	Spanish	PDF
ES 2439615	B1	20141118	Spanish	PDF
FR 2993433	A1	20140124	French	PDF
JP 2014037402	A	20140227	Japanese	PDF
US 20160338349	A1	20161124	English	PDF
US 9918465	B2	20180320	English	PDF
US 20180153162	A1	20180607	English	PDF

Chemscape – Use Cases

Search within full text of patents



The screenshot shows the Chemscape search interface. On the left, there is a sidebar with navigation icons. The main area has two tabs: "Patent" (selected) and "Structure". Below the tabs are several search filters: "All", "Abstract", "Description", "Claims", "Tit./Abs./Cla." (with a text input field containing "synergis*"), "Simple legal status" (set to "None"), "Pub. Date" (with two date pickers), and "Current Assignee". A large blue "Search" button is at the bottom, and a "Reset" link is in the bottom right corner.



The screenshot shows the search results page. At the top, there is a "< Back" link and "Results (68)" and "Patents" labels. The results are listed in a table with the following entries:

Results (68)	Patents
Tefluthrin 79538-32-2	250
(+)-Tefluthrin 391634-71-2	5
2H-1-Benzopyran-6-carboxylic acid, 3,4-dihydro-5-m... 1402549-68-1	3
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t... 411221-41-5	2
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t... 1555994-75-6	2
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t... 2115084-80-3	2
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t... 425384-10-7	2
β-D-Glucopyranuronamide, 1-(4-amino-2-oxo-1(2H)-... 1621870-06-1	2
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t... 1512845-70-3	2
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-t...	1



Chemscape – Use Cases

Analysis by assignee



L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2021 ACS on STN

[PatentPak PDF](#)

AN 2000:53333 CAPLUS [Full-text](#)

DN 132:104089

TI Synergistic insecticidal and acaricidal compositions comprising emamectin

IN Arslan-Bir, Martine

PA Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.

SO PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DT Patent

LA English

Avermectin B1, 4''-Deoxy-4''-(...
255055-56-2

[No Title]

Relative stereochemistry shown: Double bond neo

Add mark

Patent Count
1

Trade Name
-

Molecular Formula
C17H14ClF7O2.Unspecified

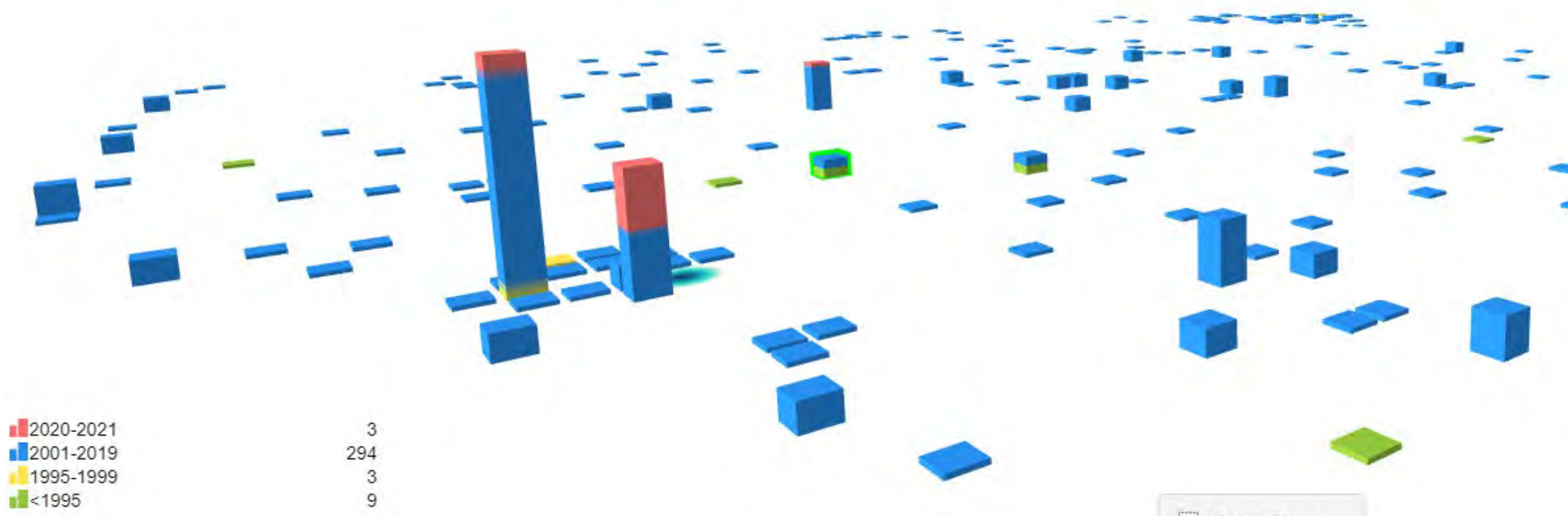
SMILES

Synonyms
Cyclopropanecarboxylic acid, 3-[(1Z)-2-chloro-3,3,3-trifluoro-1-propenyl]-2,2-dimethyl-, (2,3,5,6-tetrafluoro-4-methylphenyl)methyl ester, (1R,3R)-*re/-*, mixt. contg.

Chemscape – Use Cases

Analysis by publication year

- Identify substances indexed in expired, or very recent patents



Key takeaways

- There are different possibilities for graphical analyses within Chemscape
- Those can be used to analyze FAM, CSS or SSS structure search results to
 - Find similar substances in different/similar applications
 - Find patents based on full-text searching only for the analyzed substance answer set – review substances first before retrieving those patents
 - Get a quick overview on similar substances, patented by other assignees
 - Find substances that have very old or very recent patents

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