

CAS STNext[®] E-SEMINAR

COMPREHENSIVE PRIOR ART IN CHEMISTRY: WHAT YOU MIGHT MISS

Jim Brown, FIZ Karlsruhe







- Know your topic
- Know your tools
- Know your databases
- Develop the search strategy
- Dates, dates, dates



Know your topic

- 'Tell me what you want and I'll give you what you need' The Doobie Brothers
- A good search strategy begins with truly understanding the topic, both specifically and generally
- Learn about the background of the topic
- In-depth discussions with your requester
 - Before AND as the search is ongoing



Importance of knowing your topic

- Ability to use tools to their fullest potential
- Keywords relevant synonyms, related terms
- Classifications relevant vs. irrelevant
- Value-add tools
- Index terms/structures/sequences/polymers



Know your topic

- Do not be afraid to have ongoing conversations with requester!
- Use requester's expertise to your advantage
- When possible, use colleagues' expertise as well
- Inform requester of ongoing results/pitfalls
- Empowers requester as well



Know your tools

- Possible tools (which will vary based on search request)
- Keyword search
- Classification search
 - International Patent Classifications (IPCs)
 - Cooperative Patent Classifications (CPCs)
 - Japanese Patent Classifications (FCLs)
 - Japanese F-Terms (FTERMs)
 - European Patent Classifications (ECLA)*
 - In computer only Patent Classifications (ICOs)*
 - US Patent Classifications (NCLs)*
- * These classes have been retired but are still available in some databases for historical searching



nformation Infrastructure

Know your tools (cont.)

- Value-add abstracting
- Knowledgeable experts
- Value-add indexing
- Index terms
 - Control Terms, Supplementary Terms (CAplus)
 - Derwent Classes, Derwent Manual Codes (DWPI)
 - Specific substance indexing (CAS REGISTRY[®], Derwent Chemistry Resource (DCR), Derwent Markush Resource (DWPIM), DWPI fragmentation, ReaxysFileSub)
 - Markush indexing (MARPAT, DWPIM)
 - Sequence indexing (CAS REGISTRY, **MARPAT**, GENESEQ, **DCR**, **DWPIM**, USGENE, PATGENE)
 - Polymer indexing (CAS REGISTRY, MARPAT, Derwent World Patents Index (WPIDS, WPIX), DCR, DWPIM)



Know your tools

- Things to consider
- When did this term first come into being?
 - How would this concept have been covered before this term existed?
 - Concordances, reclassifications, back postings?
- Are there other relevant terms in that system?
 - Broader, narrower and related terms



Know your databases

- Coverage
- Country coverage
- Date coverage
 - How far back, how current
- Document coverage
 - Areas of technology, published applications, granted patents, design, plant ...
- First-level vs. value-add

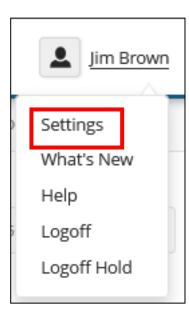


Know your tools – Keyword searching on CAS STNext using CAplus and DWPI

- Consider where to search keyword(s)
- Title, enhanced abstract(s), first level data
- May be in multiple languages
- Basic Index vs. Basic Index, Extended
- Settings associated with your STN ID
- Plurals, spellings, abbreviations
- Great tools, but beware of unforeseen consequences
- Abbreviations that have more than one meaning
- Words in another language than the one considered



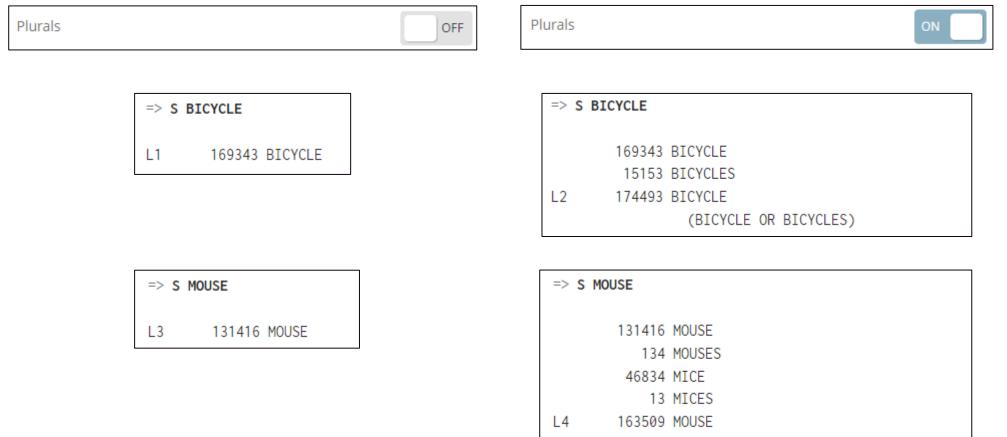
Settings



Abbreviation	ON
Audit	ON
Logoff History (LHIST)	ON
Multiple-step (Mstep)	ON
Plurals	ON
Spellings	ON
Structure Editor Toolbars	Floating 👻
Cost Notification (USD)	
Display Cost Notifications	ON
Display Cost Trigger	1
Search Cost Notifications	ON
Search Cost Trigger	1



Plurals

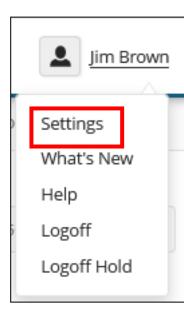


(MOUSE OR MOUSES OR MICE OR MICES)





Settings (cont.)

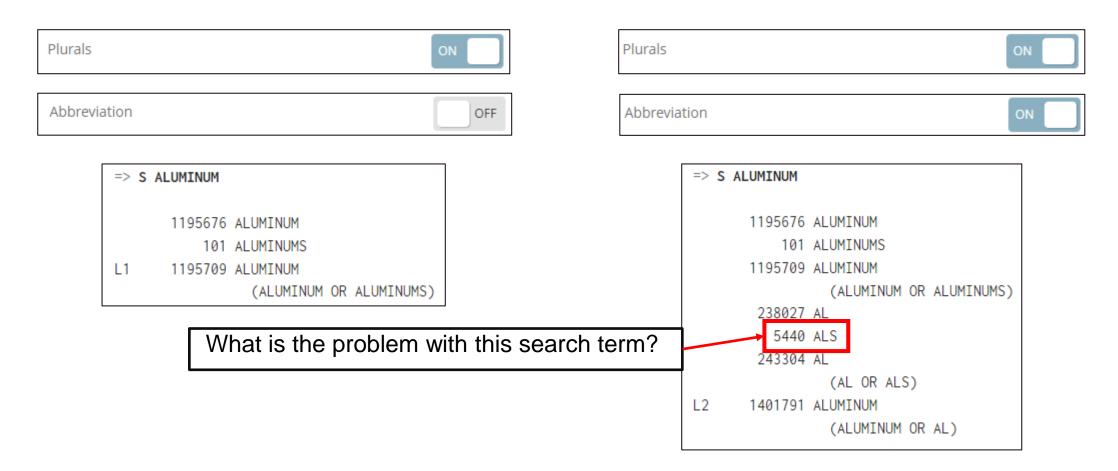


Abbreviation	ON
Audit	ON
Logoff History (LHIST)	ON
Multiple-step (Mstep)	ON
Plurals	ON
Spellings	ON
Structure Editor Toolbars	Floating 👻
Cost Notification (USD)	
Display Cost Notifications	ON
Display Cost Trigger	1
Display Cost Trigger Search Cost Notifications	1 ON



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Abbreviation







Keyword searching potential issues

=> S ALS NOT (A	ALUMINUM OR ALUMINIUM OR AL)
6052	ALS/BI
1080786	ALS/BIEX
1301247	ALUMINUM/BI
583549	ALUMINUM/BIEX
848511	ALUMINIUM/BI
1206932	ALUMINIUM/BIEX
242703	AL/BI
497871	AL/BIEX
L1 1009758	ALS/BI, BIEX NOT (ALUMINUM/BI, BIEX OR ALUMINIUM/BI, BIEX OR AL/BI,
	BIEX)

This particular search query was conducted with the plurals and abbreviations turned off.

L1	ANSWER 1 OF 1009758 WPINDEX COPYRIGHT 2023 CLARIVATE on STN
Membr	er
1 ICHION	
	einer Aussenscheibe (2), einer Innenscheibe (3) und einer
	thermoplastischen Zwischenschicht (4), (b) Ein- oder Aufbringen
	mindestens eines opaken Hintergrunds, insbesondere als opake Schicht,
	bevorzugt als Maskierungsstreifen (5,5'), in zumindest einem zweiten
	Teilbereich der innenraumseitigen Oberflaeche der Aussenscheibe (II), der





Keyword searching potential issues

L1 ANSWER 4 OF 1009758 WPINDEX COPYRIGHT 2023 CLARIVATE on STN

Member. . .

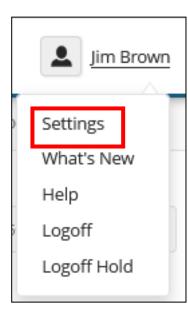
algorithm The rank of tensor RS, the value of the learning rate rn, and the tensor f by using the CP-ALS algorithm. performing decomposition to obtain initial factor matrixes S (1), S (2) and S (3); (4) constructing regularized target optimization.

L2 ANSWER 3 OF 6252 WPINDEX COPYRIGHT 2023 CLARIVATE on STN USE . . for paralyzed patients having neurological diseases. Uses include but are not limited to brainstem infarcts, brain injury, stroke and advanced amyotrophic lateral sclerosis (ALS). These types of issues are usually not a problem. When the aluminum concept is used in conjunction with other concepts, the false drops would decrease/disappear, but the experienced searcher would keep an eye on this type of issue.





Settings (cont.)

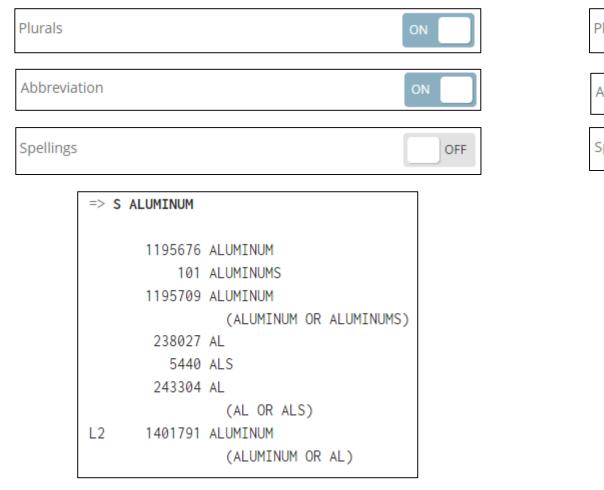


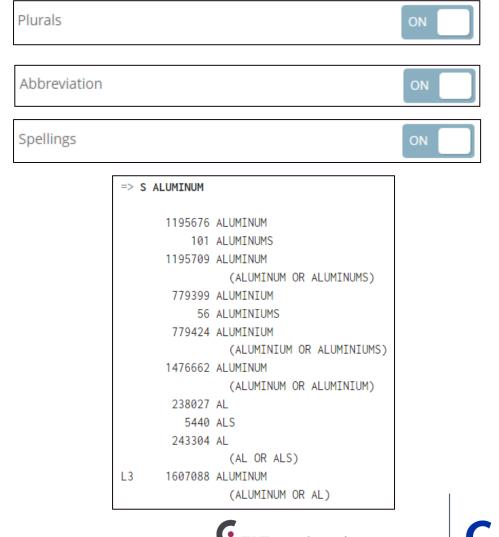
Abbreviation	ON
Audit	
Logoff History (LHIST)	ON
Multiple-step (Mstep)	ON
Plurals	ON
Spellings	ON
Structure Editor Toolbars	Floating 👻
Cost Notification (USD)	
Display Cost Notifications	ON
Display Cost Trigger	1
Search Cost Notifications	ON
Search Cost Trigger	1



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Spellings

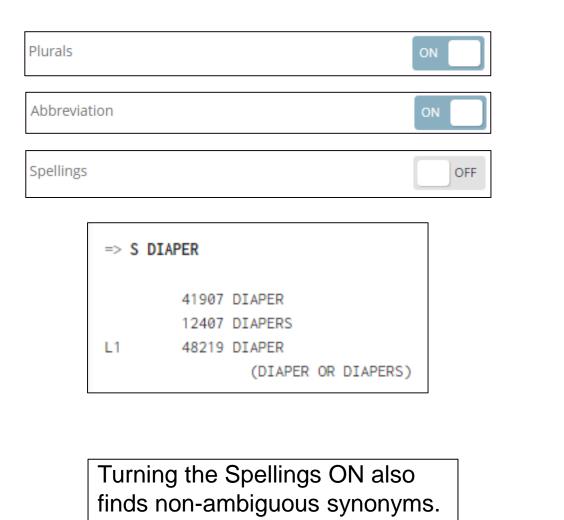


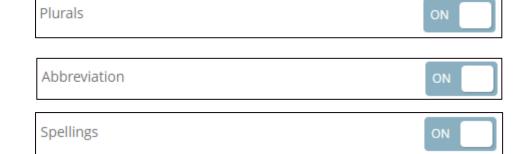


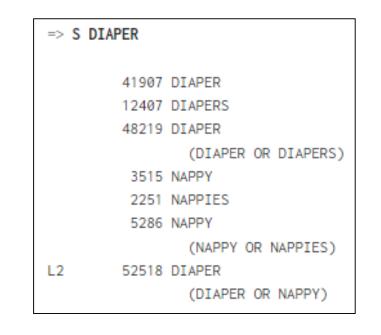




Spellings











Basic Index

- Search a keyword without a search qualifier, the system will search the 'basic index' of that database
- The basic index changes from database to database
- Most searches require the searcher to tell the system where to look, by using a search qualifier
 - Inventors /IN
 - Assignees /PA





Basic index for DWPI

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains single words from AB, ABDT, ABEQ, ABEX, ACTN, ACTV, ADV, ALE, DETD, DRWD, NOV, TECH, TI, TT, UADV, and USE) (18)	None or /BI (or /BIX)	S DRILLING FLUID AND EMULS? S ?PHENYLETHER? S #####DIPHENYLETHER S ULCER TREATMENT(L)ORAL	AB, ABDT, ABEQ, ABEX, ACTN, ACTV, ADV, ALE, DETD, DRWD, NOV, TECH, TI, TT, UADV, USE

- Value-add data
- Derwent enhanced titles and abstracts
- Search with no search qualifier or with /BI search qualifier





Basic index Extended for DWPI

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index Extended* (contains single terms from author abstracts, claims, and original titles) (2)	/BIEX	S NANOCLUSTERS/BIEX	ABDE, ABEN, ABES, ABFR, ABOL, CLMDE, CLMEN, CLMES, CLMFR, CLMOL, TIDE, TIEN, TIES, TIFR, TIOL

- Available first level data
- ~ 20 patent authorities
- Original titles, original abstracts, claims
- Search with /BIEX search qualifier
- To have the system search both fields permanently, use the command SET SFIELDS BI BIEX PERM





BI and BIEX keyword search in DWPI

=> S ALUMINUM SET COMMAND COMPLETED 1195676 ALUMINUM 101 ALUMINUMS => S ALUMINUM 1195709 ALUMINUM (ALUMINUM OR ALUMINUMS) 779399 ALUMINIUM 56 ALUMINIUMS 779424 ALUMINIUM (ALUMINIUM OR ALUMINIUMS) 1476662 ALUMINUM (ALUMINUM OR ALUMINIUM) 238027 AL 5440 ALS 243304 AL (AL OR ALS) L3 1607088 ALUMINUM (ALUMINUM OR AL)

=> SET SFIELDS BI BIEX PERM 1195676 ALUMINUM/BI 101 ALUMINUMS/BI 1195709 ALUMINUM/BI ((ALUMINUM OR ALUMINUMS)/BI) 779399 ALUMINIUM/BI 56 ALUMINIUMS/BI 779424 ALUMINIUM/BI ((ALUMINIUM OR ALUMINIUMS)/BI) 1476662 ALUMINUM/BI ((ALUMINUM OR ALUMINIUM)/BI) 238027 AL/BT 5440 ALS/BI 243304 AL/BT ((AL OR ALS)/BI) 1607088 ALUMINUM/BI ((ALUMINUM OR AL)/BI)

555337 ALUMINUM/BIEX 140 ALUMINUMS/BIEX 555375 ALUMINUM/BIEX ((ALUMINUM OR ALUMINUMS)/BIEX) 1072697 ALUMINIUM/BIEX 815 ALUMINIUMS/BIEX 1072952 ALUMINIUM/BIEX ((ALUMINIUM OR ALUMINIUMS)/BIEX) 1403137 ALUMINUM/BIEX ((ALUMINUM OR ALUMINIUM)/BIEX) 456363 AL/BIEX 1058977 ALS/BIEX 1487629 AL/BIEX ((AL OR ALS)/BIEX) 2779659 ALUMINUM/BIEX ((ALUMINUM OR AL)/BIEX) 3319907 ALUMINUM/BI, BIEX



4



Basic index for CAplus

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index * (contains single words from title (TI), supplementary term (ST), index term (IT), and abstract (AB) fields, as well as CAS Registry Numbers)	None (or /Bl or /IA)	S 50-21-5 S TRANSGENIC COTTON S ?FLUOROCARBON? S (WATER(S)OIL)/BI	AB, IT, ST, TI

- Value-add data

- CAS enhanced titles, abstracts and index terms
- Search with no search qualifier or with /BI search qualifier





Basic index Extended for CAplus

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index * (contains single words from title (TI), supplementary term (ST), index term (IT), and abstract (AB) fields, as well as CAS Registry Numbers)	None (or /BI or /IA)	S 50-21-5 S TRANSGENIC COTTON S ?FLUOROCARBON? S (WATER(S)OIL)/BI	AB, IT, ST, TI
Basic Index plus Claims *	/BI,BIEX or /BI,CLM	S ALLOPURINOL/BI,BIEX S TRANSGENIC/BI,CLM(W)COTTON/BI,CLM	BIB CLM ALL CLM

- Original claims

- Search with /BIEX search qualifier
- To have the system search both fields permanently, use the command SET SFIELDS BI BIEX PERM





Classifications

- All of the current classification schemes get updated
- Older records may get reclassified
- Classification concordances
 - i.e., <u>CPC Concordances | Cooperative Patent Classification</u> covers ECLA to CPC and CPC to IPC
- Retired classification schemes do not get updated but may still be useful
- JP classifications unique to JP documents, may provide additional search results



Classifications (cont.)

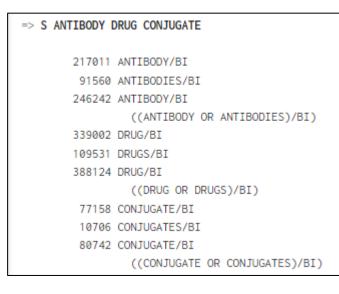
- To find relevant classifications
- Create preliminary search set
 - -Keyword search, other tools
- ANALYZE set by classification scheme(s) of interest
- Use CAS STNext classification thesauri to determine quality of term
 - Consider Broader, Narrower, Related Terms



Classification example

- This example was run in Derwent World Patents Index database
- Plurals, abbreviations and spellings on
- Search fields are the basic index and the basic index extended

L1



2588 ANTIBODY DRUG CONJUGATE/BI ((ANTIBODY(W)DRUG(W)CONJUGATE)/BI) 171692 ANTIBODY/BIEX 73873 ANTIBODIES/BIEX 194741 ANTIBODY/BIEX ((ANTIBODY OR ANTIBODIES)/BIEX) 366856 DRUG/BIEX 77730 DRUGS/BIEX 401188 DRUG/BIEX ((DRUG OR DRUGS)/BIEX) 80065 CONJUGATE/BIEX 16867 CONJUGATES/BIEX 86445 CONJUGATE/BIEX ((CONJUGATE OR CONJUGATES)/BIEX) 2985 ANTIBODY DRUG CONJUGATE/BIEX ((ANTIBODY(W)DRUG(W)CONJUGATE)/BIEX) 3292 ANTIBODY DRUG CONJUGATE/BI, BIEX

The abbreviation ADC was not created by the system, nor was it included in the search strategy as it gave a lot of false drops. For example, ADC also stands for analog to digital converter.

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ANALYZE the CPCs and IPCs

=> ANALYZE L1 IPC CPC 1-3292

L2 ANALYZE L1 1-3292 IPC CPC : 5728 TERMS

=> D CPC 1-

View all

TERM #	# OCC	# DOC	% DOC	IPC CPC
5	2018	1592	48.36	A61P0035-00
8	1482	1076	32.69	A61K0047-6803
10	1057	281	8.54	A61K2300-00
11	1053	861	26.15	A61K2039-505
13	1045	773	23.48	A61K0047-6849
18	742	623	18.92	C07K2317-24
20	723	589	17.89	A61K0047-6851
22	678	563	17.10	C07K2317-92
23	655	500	15.19	A61K0045-06
24	646	489	14.85	A61K0047-6889
30	572	486	14.76	C07K2317-565
33	453	353	10.72	C07K0016-30
34	442	382	11.60	C07K2317-73
36	417	342	10.39	C07K2317-76
37	412	324	9.84	C07K0016-32
40	407	303	9.20	C07K0016-28
41	405	315	9.57	A61K0047-6855
45	357	259	7.87	C07K0016-2803
48	345	207	6.29	A61K0039-39558

. . .

TERM #	# OCC	# DOC	% DOC IPC CPC
1	4528	2305	70.02 A61P0035-00
2	4165	2024	61.48 A61K0047-68
3	3674	1656	50.30 C07K0016-28
4	3515	1839	55.86 A61K0039-395
6	1815	981	29.80 A61K0039-00
7	1503	833	25.30 C07K0016-30
9	1092	692	21.02 C12N0015-13
12	1051	482	14.64 A61K0047-48
14	935	604	18.35 A61K0045-06
15	821	599	18.20 A61P0035-02
16	813	725	22.02 A61K0045-00
17	750	524	15.92 C07K0016-46
19	740	450	13.67 C07K0016-00
21	701	607	18.44 A61P0043-00
25	646	460	13.97 C07K0019-00
26	614	392	11.91 C07K0016-18
27	601	360	10.94 C07K0016-32
28	582	361	10.97 G01N0033-574
29	573	465	14.13 C12N0005-10

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Use the CAS STNext Thesauri

- The command to access the various thesauri
- EXPAND term + ALL/IPC or
- EXPAND term +ALL/CPC

=> E A61P0035-00+ALL/CPC					
E1	0	BT4	A/CPC		
			HUMAN NECESSITIES(2013-01-01)		
E2	0	BT3	A6/CPC		
			HEALTH; AMUSEMENT(2013-01-01)		
E3	0	BT2	A61/CPC		
			MEDICAL OR VETERINARY SCIENCE; HYGIENE(2013-01-01)		
E4	420755	BT1	A61P/CPC		
			SPECIFIC THERAPEUTIC ACTIVITY OF CHEMICAL COMPOUNDS OR		
			MEDICINAL PREPARATIONS(2018-01-01)		
E5	116694	>	A61P0035-00/CPC		
			Antineoplastic agents(2018-01-01)		
E6	18371	NT1	A61P0035-02/CPC		
			specific for leukemia(2018-01-01)		
E7	10378	NT1	A61P0035-04/CPC		
			specific for metastasis(2018-01-01)		
*****	***** END *******				

This was the highest posted class in both the IPCs and CPCs, but may not be the best class code for this concept.

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Use the CAS STNext Thesauri

=> E A61K0047-68+ALL/CPC			E9	300	NT1	A61K0047-6801/CPC	
							CPC-specific-text: Drug-antibody or immunoglobulin
E1	0	BT7	A/CPC				conjugates defined by the pharmacologically or
			HUMAN NECESSITIES(2013-01-01)				therapeutically active agent(2017-08-01)
E2	0	BT6	A6/CPC	E10	2520	NT2	A61K0047-6803/CPC
			HEALTH; AMUSEMENT(2013-01-01)				CPC-specific-text: Drugs conjugated to an antibody or
E3	0	BT5	A61/CPC				immunoglobulin, e.g. cisplatin-antibody
			MEDICAL OR VETERINARY SCIENCE; HYGIENE(2013-01-01)				conjugates(2017-08-01)
E4	809041	BT4	A61K/CPC	E11	55	NT3	A61K0047-6805/CPC
			PREPARATIONS FOR MEDICAL, DENTAL, OR TOILET PURPOSES				CPC-specific-text: the drug being a vinca
			reference: devices or methods specially adapted for				alkaloid(2017-08-01)
			bringing pharmaceutical products into particular	E12	318	NT3	A61K0047-6807/CPC
			physical or administering forms A61J0003-00;				CPC-specific-text: the drug or compound being a sugar,
E5	671	BT3	A61K0047-00/CPC				nucleoside, nucleotide, nucleic acid, e.g. RNA
			Medicinal preparations characterised by the non-active				antisense(2017-08-01)
			ingredients used, e.g. carriers or inert	E13	438	NT4	A61K0047-6809/CPC
			additives;Targeting or modifying agents chemically bound				CPC-specific-text: Antibiotics, e.g. antitumor
			to the active ingredient(2017-08-01)				antibiotics anthracyclins, adriamycin, doxorubicin or
E6	1704	BT2	A61K0047-50/CPC				daunomycin(2017-08-01)
			the non-active ingredient being chemically bound to the	E14	891	NT3	A61K0047-6811/CPC
			active ingredient, e.g. polymer-drug				CPC-specific-text: the drug being a protein or peptide,
			conjugates(2017-08-01)				e.g. transferrin or bleomycin(2017-08-01)
E7	147	BT1	A61K0047-51/CPC	E15	361	NT4	A61K0047-6813/CPC
			the non-active ingredient being a modifying				CPC-specific-text: the drug being a peptidic cytokine,
			agent(2017-08-01)				e.g. an interleukin or interferon(2017-08-01)
E8	928	>	A61K0047-68/CPC	E16	188	NT4	A61K0047-6815/CPC
			the modifying agent being an antibody, an immunoglobulin				CPC-specific-text: Enzymes(2017-08-01)
			or a fragment thereof, e.g. an Fc-fragment(2017-08-01)				

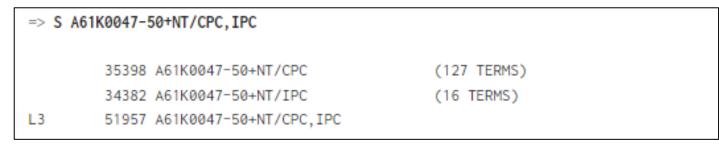
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Classification discussion

- These classes look much better, but what is the right level to use?
- Broader/narrower than the term expanded around?
- To include all narrower classes plus the class in question in both the IPC and CPC systems, use
- S class+NT/IPC,CPC
- For this example, the class for E5 is used as the broadest level
- SA61K0047-50+NT/CPC,IPC





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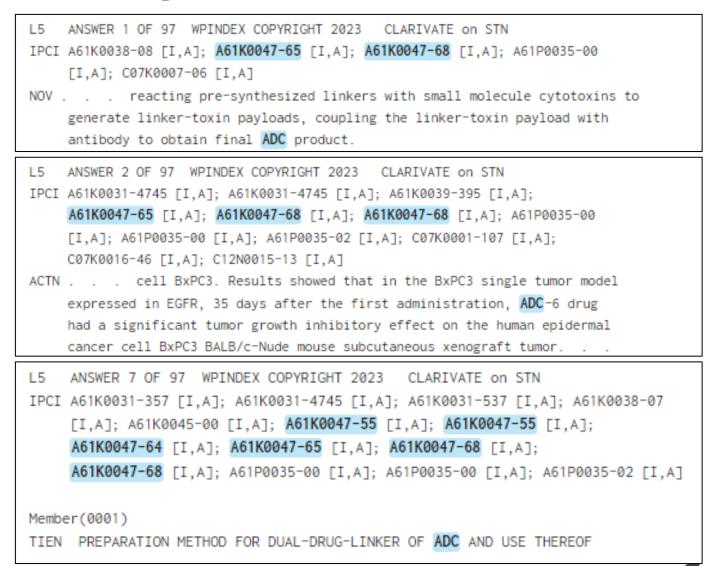
Classifications

 Now the ADC abbreviation can be used in conjunction with the class set

=> S ADC AND	L3
2611	7 ADC/BI
157	6 ADCS/BI
2672	6 ADC/BI
	((ADC OR ADCS)/BI)
4671	2 ADC/BIEX
240	9 ADCS/BIEX
4728	1 ADC/BIEX ((ADC OR ADCS)/BIEX)
L4 102	2 ADC/BI,BIEX AND L3
=> s 14 not 1	1
L5 9	7 L4 NOT L1



Unique ADC plus class results





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Include Japanese classification codes

=> S A61K0047-50/FCL L6 1872 A61K0047-50/FCL => S L6 NOT L3 L7 841 L6 NOT L3 => D TI PI 1-2 ANSWER 1 OF 841 WPINDEX COPYRIGHT 2023 CLARIVATE on STN L7 New tamoxifen compound used in pharmaceutical composition for treating TI cancer e.g. stomach cancer, colon cancer, liver cancer, pancreatic cancer, lung cancer and breast cancer, multiple myeloma, amyloidosis and autoimmune disease A 20161228 (201708) * JA 82[9] JP 2016222659 ΡI B2 20201125 (2020096) JA 82 JP 6792256 ANSWER 2 OF 841 WPINDEX COPYRIGHT 2023 CLARIVATE on STN L7 New fusion protein comprises fusion of bone morphogenetic protein 7 (BMP7) TI variant and human serum albumin, useful for preparing therapeutic agent for renal disease A 20161208 (201701) * JA 12[9] ΡI JP 2016204292

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- Value-add searching
- Understand basic indexing principles
- Understand indexing tools available to indexer



Derwent World Patents Index

- The Derwent World Patents Index database (DWPI) is the main/ultimate Derwent database
- Patent family database
- Value add abstracting, manual codes, Derwent classes, polymer indexing
- DCR and DWPIM indexing with roles
- Fragmentation
- Citation info



Derwent companion databases

- Derwent Chemistry Resource (DCR)
- Specific compounds +
- 1999, plus some earlier
- Derwent Markush Resource (DWPIM)
- Markush structures
- Specific compounds
- ~ 1978, plus some earlier



Derwent indexing of small molecules

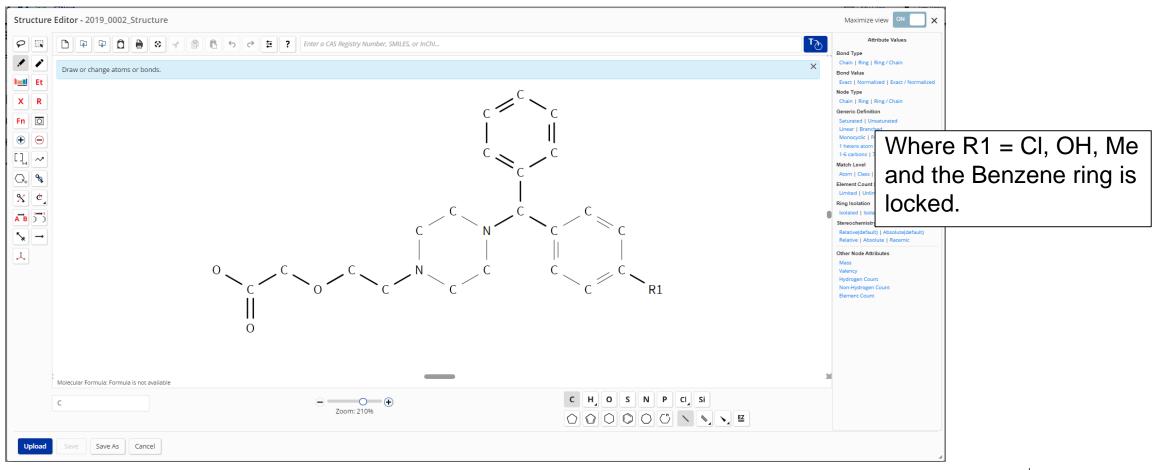
- Fragmentation 1963 -
- Derwent Markush Resource (DWPIM) ~1978 -
- Derwent Chemistry Resource (DCR) ~1999 –
- Some earlier indexing DCNs and DRNs
- To cover all time periods, fragmentation must be included!



Derwent small molecule search

- Draw structure
- Structure search in DCR
- Structure search in DWPIM
- S DCR set and DWPIM set in DWPI to get patent family records
- Run frag search, find unique records







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File DCR =>	=> FILE DCR
Uploading structure file: 2019_0002_Structure	
	=> S L1 SSS FULL
.35	
	FULL SEARCH INITIATED 11:14:46
	FULL SCREEN SEARCH COMPLETED - 5204481 TO ITERATE
	100.0% PROCESSED 5204481 ITERATIONS 87 ANSWERS
	SEARCH TIME: 00.00.02
0 12	
	L2 87 SEA SSS FUL L1
R-Group Definitions	=> FILE DWPIM
R1: C1,OH,Me	
Node Attributes	
Ring Nodes : 2 3 4 5 13 14 15 16 17 18 20 21 22 23 24 25 26 27	=> S L1 SSS FULL
Isolated Ring Nodes : 22 23 24 25 26 27	
Chain Nodes : 1 6 7 8 9 10 11 12	
Bond Attributes	100.0% PROCESSED 2638066 ITERATIONS (1 INCOMPLETE) 59 ANSWERS
Ring Bonds : 2-3 2-14 3-4 4-5 13-5 14-13 15-16 15-21 16-17 17-18 20-18 21-20 22-23 22-27 23-24 24-25 26-25 27-26 Chain Bonds : 1-2 1-15 1-22 5-6 6-7 7-8 8-9 9-10 10-11 10-12 18-19	
Normalized Bonds : 15-16 15-21 16-17 17-18 20-18 21-20 22-23 22-27 23-24 24-25 26-25 27-26	SEARCH TIME: 00.03.03
Exact/Normalized Bonds : 1-2 1-15 1-22 2-3 2-14 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 10-12 13-5 14-13 18-19	
Markush Attributes	L3 59 SEA SSS FUL L1
Match Level (ATOM) : 2 3 4 5 13 14 15 16 17 18 20 21 22 23 24 25 26 27	L3 59 SEA SSS FUL L1
Match Level (CLASS) : 1 6 7 8 9 10 11 12	
Element Count Level (LIMITED) : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 20 21 22 23 24 25 26 27	
L1 STRUCTURE UPLOADED	

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=> FILE WPIX; S L2; S L3	=> D 1-3	36				18	43	43	3.25 2016
-> TILL MIX, 3 L2, 3 L3						19	42	42	3.17 2023
	L7	ANA	LYZE L6	1- PY.B :	36 TERMS	20	41	41	3.09 2015
L4 1313 L2	TERM #	# 000	# DOC	% DOC PY.B		21	38	38	2.87 2004
		# 000	# DOC			22	25	25	1.89 2002
	1	99	99	7.47 2009		23	17	17	1.28 2001
	2	84	84	6.34 2022		24	16	16	1.21 1999
L5 38 L3	3	83	83	6.26 2010		25	10	10	0.75 2000
	4	72	72	5.43 2007		26	9	9	0.68 1997
=> S L4 OR L5	5	65	65	4.91 2008		27	8	8	0.60 1998
	6	65	65	4.91 2021		28	6	6	0.45 1995
L6 1325 L4 OR L5	7	60	60	4.53 2014		29	4	4	0.30 1994
	8	59 58	59 58	4.45 2019 4.38 2011		30	3	3	0.23 1988
=> ANA PY.B L6 1-	10	55	55	4.15 2013		31	3	3	0.23 1990
	11	55	55	4.15 2020		32	2	2	0.15 1992
	12	54	54	4.08 2012		33	2	2	0.15 1993
ANALYZE IS APPROXIMATELY 64% COMPLETE	13	52	52	3.92 2005		34	2	2	
L7 ANALYZE L6 1- PY.B : 36 TERMS	14	52	52	3.92 2017		35	1	1	0.08 1989
	15	52	52	3.92 2018		36	1	1	0.08 1991
	16	44	44	3.32 2003		*******	END OF	E L 7	*******
	17	/13	13	3 25 2006			2		

17

43

43 3.25 2006

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 Return to Session Structures (152) 		S	iort: Date Modified: Newest 🗸
Move to Folder Search F	iles by Name	Q Import Sequen	ce [f] Import Structure
2019_0002_Structure 14 Nov 2023 11:14 AM			← Upload Move Delete Download Generate FragCode Script
			Generate Derwent fra



Edit Script	×
2019_0002_Structure_FragCode_01 Check your script with the validate button.	
Save As	Validation
1 =>s (H602)/M0,M2,M3,M4 \>_line1	Success
<pre>2 =>s _line1(P)(M322)/M0,M2,M3,M4 \>_line2 3 =>s _line2(P)(H641)/M0,M2,M3,M4 \>_line3 4 =>s (_line1(P)M900/M0) OR (_line1(P)M901/M2,M3,M4) OR (_line2(P)M902/M2,M3,M4) OR _line3 \>_line4 5 =>s _line4(NOTP)(H4 OR H7)/M2,M3,M4 \>_line5 6 =>s (H401(P)H441)/M0,M2,M3,M4 \>_line6 7 =>s _line6(P)(M322)/M0,M2,M3,M4 \>_line7 8 =>s (_line6(P)M900/M0) OR (_line6(P)M901/M2,M3,M4) OR (_line7(P)M902/M2,M3,M4) OR _line7 \>_line8 9 =>s _line8(NOTP)(H6 OR H7)/M2,M3,M4 \>_line9 10 =>s (H721(P)M341)/M0,M2,M3,M4 \>_line10 11 =>s _line10(P)(M323)/M0,M2,M3,M4 \>_line11</pre>	No errors detected
<pre>12 =>s (_line10(P)M900/M0) OR (_line10(P)M901/M2,M3,M4) OR (_line11(P)M902/M2,M3,M4)</pre>	
Run Save Cancel	

Run the search as is, unedited, which means this is NOT a true substructure search.





- => s (H602)/M0,M2,M3,M4
 - 16791 (H602)/M0
 - 335425 (H602)/M2
 - 167468 (H602)/M3
 - 48104 (H602)/M4
- L8 533746 (H602)/M0,M2,M3,M4
- => s L8(P)(M322)/M0,M2,M3,M4
 - 32433 (M322)/M0
 - 418011 (M322)/M2
 - 337872 (M322)/M3
 - 59774 (M322)/M4
- L9 218285 L8(P)(M322)/M0,M2,M3,M4
- => s L9(P)(H641)/M0,M2,M3,M4
 - 473934 K0/M3
 - 65708 K0/M4
- L28 1408 L27(NOTP)(H3 OR H9 OR J2 OR J3 OR J4 OR J5 OR J9 OR K0)/M2,M3,M4

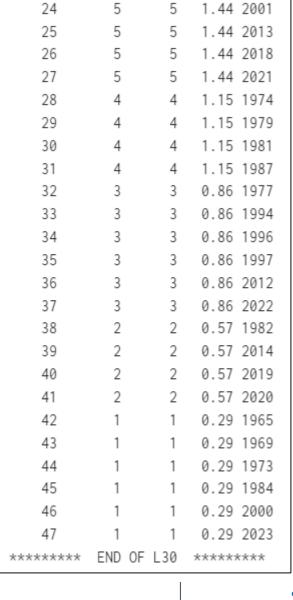




=> S L28 N0	DT L6	
L29	348 L28 NOT L6	
=> ANA PY.E	3 L29 1-348	
L30	ANALYZE L29 1-348 PY.B :	47 TERMS
=> D 1-47		
View all		

26					
27	PY.B	% DOC	# DOC	# OCC	TERM #
28	 				
29	1989	5.46	19	19	1
30	1988	5.17	18	18	2
31	2005	5.17	18	18	3
32	2007	5.17	18	18	4
33	2004	4.02	14	14	5
34	2002	3.74	13	13	6
35	2006	3.74	13	13	7
36		3.45		12	8
37		3.45		12	9
38	1991	3.16	11	11	10
	2010	3.16	11	11	11
39	1992	2.59	9	9	12
40	2003	2.59	9	9	13
41	1976	2.30	8	8	14
42	2011	2.01	7	7	15
43	1990	1.72	6	6	16
44	1999	1.72	6	6	17
45	1975	1.44	5	5	18
46	1983	1.44	5	5	19
47	1985	1.44	5	5	20
*******		1.44	5	5	21
		1.44		5	22
	1995	1.44	5	5	23

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Polymers indexed in the Derwent databases

- Derwent has two polymer indexing systems in DWPI
- Derwent enhanced polymer indexing
- Derwent Plasdoc indexing (retires system but required for backfile searching)
- However, some polymer indexing can be found in DCR and DWPIM
- The polymer itself, or monomers, or modifiers

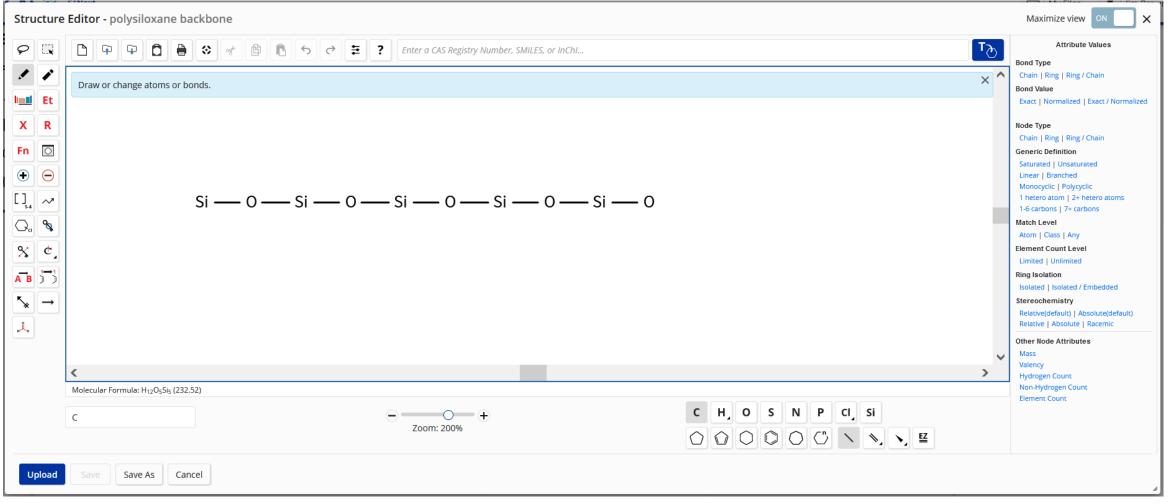


Polymers indexed in the CAS databases

- CAS has one polymer indexing system
- Monomer-based indexing
- Structural repeating units (SRUs)
- However, some polymer indexing can be found in MARPAT
- The polymer itself, or monomers, or modifiers



Sample polymeric structure





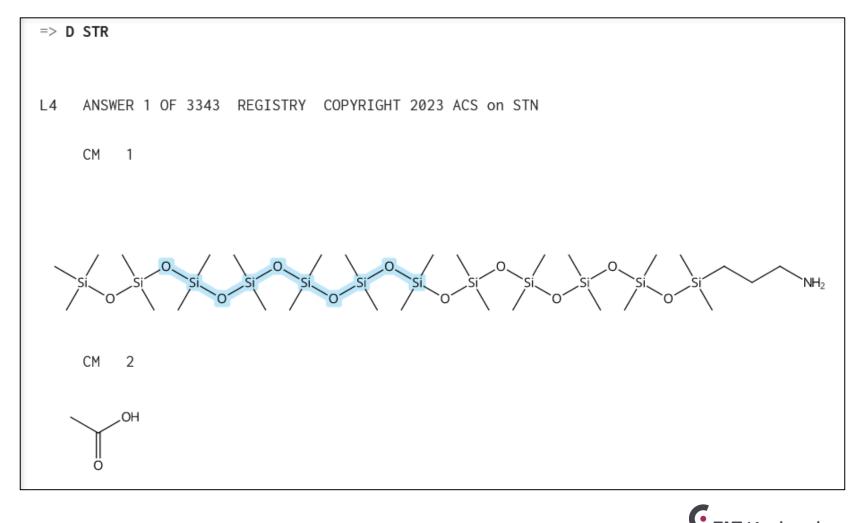


Substructure Searching polymeric structure in CAS REGISTRY

=> s l1 sss full	
FULL SEARCH INITIATED 11:38:10 FULL SCREEN SEARCH COMPLETED - 48285 TO ITERATE	
100.0% PROCESSED 48285 ITERATIONS SEARCH TIME: 00.00.01	3343 ANSWERS
L4 3343 SEA SSS FUL L1	



Substructure Searching polymeric structure in CAS REGISTRY





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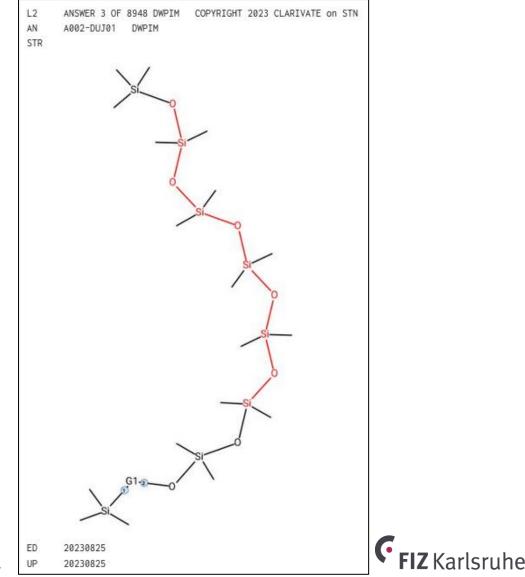
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Substructure Searching polymeric structure in DWPIM

L1 STRUCTURE UPLOADED	
=> s l1 sss full	
FULL SEARCH INITIATED 11:30:59 FULL SCREEN SEARCH COMPLETED - 2634767 TO ITERATE	
100.0% PROCESSED 2634767 ITERATIONS SEARCH TIME: 00.00.02	8948 ANSWERS
L2 8948 SEA SSS FUL L1	
=> d 3	



Substructure Searching polymeric structure in DWPIM



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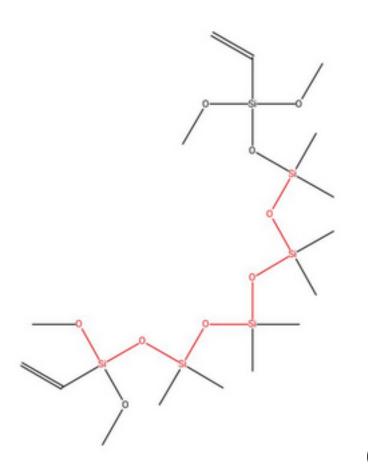
Substructure Searching polymeric structure in DCR

=> s l1 sss full	
FULL SEARCH INITIATED 11:34:16 FULL SCREEN SEARCH COMPLETED - 5187375 TO ITERATE	
100.0% PROCESSED 5187375 ITERATIONS SEARCH TIME: 00.00.03	282 ANSWERS
L3 282 SEA SSS FUL L1	



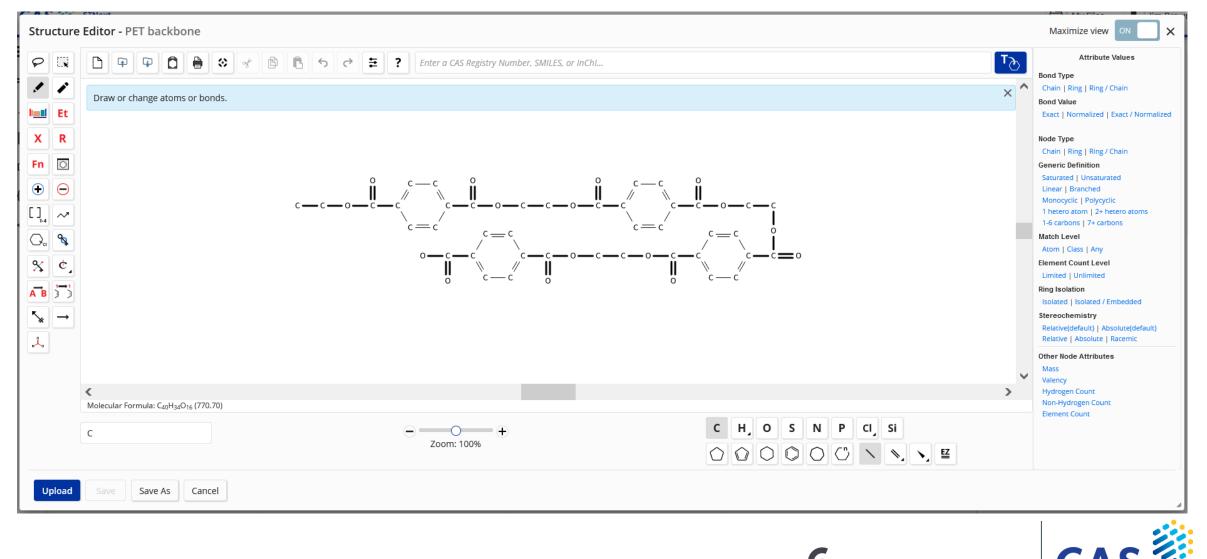
Substructure Searching polymeric structure in DCR (cont.)

- AN DCR-5993231 DCR
- DCSE 5993231-8-8-0
- CN.P 3,13-dietheryl-3,13-dimethoxy-5,5,7,7,9,9,11,11-octamethyl-2,4,6,8,10,12,14-heptacxa-3,5,7,9,11,13-hexasilapentadecane
- STR





PET polymer backbone



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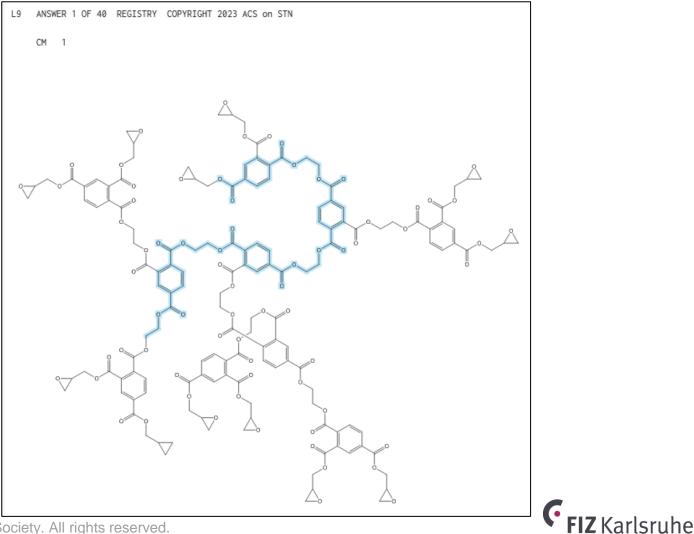
American Chemical Society

Substructure searching PET polymeric structure in CAS REGISTRY

=> S L6 SSS FULL	
FULL SEARCH INITIATED 12:24:52 FULL SCREEN SEARCH COMPLETED - 3112 TO ITERATE	
100.0% PROCESSED 3112 ITERATIONS SEARCH TIME: 00.00.01	40 ANSWERS
L9 40 SEA SSS FUL L6	



Substructure searching PET polymeric structure in CAS REGISTRY (cont.)





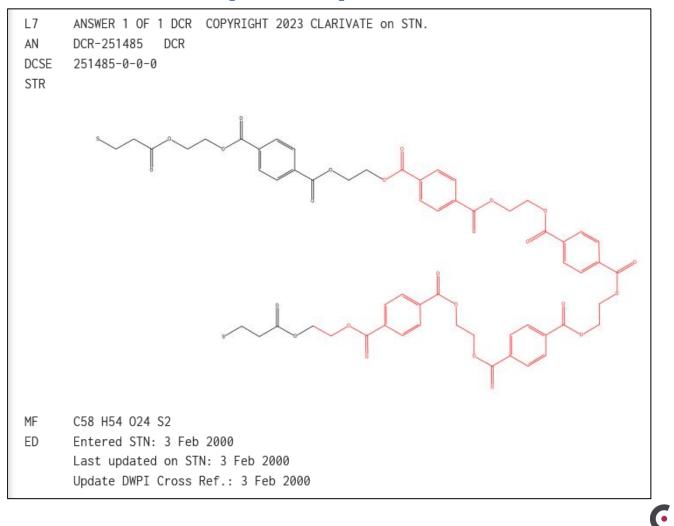
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Substructure searching PET polymeric structure in DCR

L6 STRUCTURE UPLOADED	
=> S L6 SSS FULL	
FULL SEARCH INITIATED 12:04:45 FULL SCREEN SEARCH COMPLETED - 5187375 TO ITERATE	
100.0% PROCESSED 5187375 ITERATIONS SEARCH TIME: 00.00.02	1 ANSWERS
L7 1 SEA SSS FUL L6	



Substructure searching PET polymeric structure in DCR (cont.)





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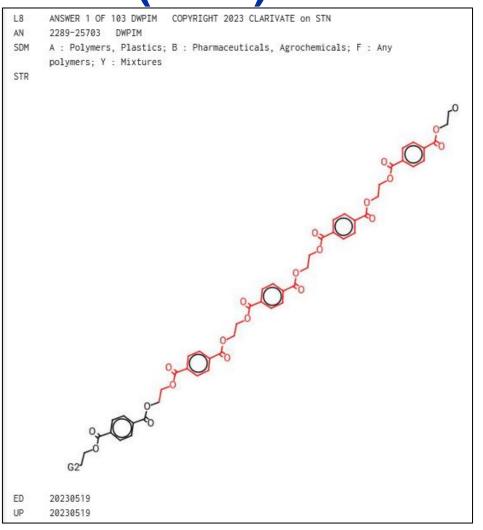
FIZ Karlsruhe

Substructure searching PET polymeric structure in DWPIM

=> S L6 SSS FULL	
FULL SEARCH INITIATED 12:19:10 FULL SCREEN SEARCH COMPLETED - 2634767 TO ITERATE	
100.0% PROCESSED 2634767 ITERATIONS SEARCH TIME: 00.00.34	103 ANSWERS
L8 103 SEA SSS FUL L6	



Substructure searching PET polymeric structure in DWPIM (cont.)







Sequence searching

- CAS REGISTRY
- BLAST, Motif and Structure searching
- GENESEQ, USGENE, PATGENE
- BLAST, and Motif searching
- DCR
- Structure searching
- Chemical Name/Chemical Name Segment
- DWPIM/MARPAT



CAS REGISTRY record for Humira

L2	ANSWER 1 OF 1 REGISTRY COPYRIGHT 2023 ACS on STN			
RN	331731-18-1 REGISTRY			
ED	Entered STN: 18 Apr 2001			
CN	Immunoglobulin G1, anti-(human tumor necrosis factor) (human monoclonal			
	D2E7 heavy chain), disulfide with human monoclonal D2E7 light chain, dimer			
	(CA INDEX NAME)			
OTHE	ER NAMES:			
CN	Adalimumab			
CN	Adalimumab-aqvh			
CN	Adalimumab-CinnaGen			
CN	CHS-1420			
CN	CinnoRA			
CN	D 2E7			
CN	D2E7			
CN	Humira			
CN	LU 200134			
CN	Yusimry			
FS	PROTEIN SEQUENCE			
SQL	1330,451,451,214,214			
NTE	multichain			





CAS REGISTRY record for Humira (cont.)

SEQ1EVQLVESGGGLVQPGRSLRLSCAASGFTFDDYAMHWVRQAPGKGLEWVSA51ITWNSGHIDYADSVEGRFTISRDNAKNSLYLQMNSLRAEDTAVYYCAKVS101YLSTASSLDYWGQGTLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLV151KDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQ201TYICNVNHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPK251PKDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQY301NSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREP351QVYTLPPSRDELTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPP401VLDSDGSFFLYSKLTVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPG451KKKKKK

SEQ1EVQLVESGGGLVQPGRSLRLSCAASGFTFDDYAMHWVRQAPGKGLEWVSA51ITWNSGHIDYADSVEGRFTISRDNAKNSLYLQMNSLRAEDTAVYYCAKVS101YLSTASSLDYWGQGTLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLV151KDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQ201TYICNVNHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPK251PKDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQY301NSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREP351QVYTLPPSRDELTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPP401VLDSDGSFFLYSKLTVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPG451KKKKKK

SEQ	1	DIQMTQSPSS	LSASVGDRVT	ITCRASQGIR	NYLAWYQQKP	GKAPKLLIYA	
	51	ASTLQSGVPS	RFSGSGSGTD	FTLTISSLQP	EDVATYYCQR	YNRAPYTFGQ	
	101	GTKVEIKRTV	AAPSVFIFPP	SDEQLKSGTA	SVVCLLNNFY	PREAKVQWKV	
	151	DNALQSGNSQ	ESVTEQDSKD	STYSLSSTLT	LSKADYEKHK	VYACEVTHQG	
	201	LSSPVTKSFN	RGEC				
SEQ	1	DIQMTQSPSS	LSASVGDRVT	ITCRASQGIR	NYLAWYQQKP	GKAPKLLIYA	
	51	ASTLQSGVPS	RFSGSGSGTD	FTLTISSLQP	EDVATYYCQR	YNRAPYTFGQ	
	101	GTKVEIKRTV	AAPSVFIFPP	SDEQLKSGTA	SVVCLLNNFY	PREAKVQWKV	
	151	DNALQSGNSQ	ESVTEQDSKD	STYSLSSTLT	LSKADYEKHK	VYACEVTHQG	

201 LSSPVTKSFN RGEC

Derwent indexing for Humira

- Sequences in individual GENESEQ records
- TRANSFER PNs from each GENESEQ search into DWPI, AND the two sets
- Check DCR
 - Structure?
 - Name/name segment?
 - Subject descriptor/Comment field?



Humira heavy chain

Edit Biosequence	×
Humira heavy chain 🏒	
Check your sequence with the Validate button.	
Save As 🗗 🗊 🔿 C Validate	Validation
1 1 EVQLVESGGG LVQPGRSLRL SCAASGFTFD DYAMHWVRQA PGKGLEWVSA	
2 51 ITWNSGHIDY ADSVEGRFTI SRDNAKNSLY LQMNSLRAED TAVYYCAKVS	
3 101 YLSTASSLDY WGQGTLVTVS SASTKGPSVF PLAPSSKSTS GGTAALGCLV 4 151 KDYFPEPVTV SWNSGALTSG VHTFPAVLQS SGLYSLSSVV TVPSSSLGTQ	
201 TYICNVNHKP SNTKVDKKVE PKSCDKTHTC PPCPAPELLG GPSVFLFPPK	
6 251 PKDTLMISRT PEVTCVVVDV SHEDPEVKFN WYVDGVEVHN AKTKPREEQY	
7 301 NSTYRVVSVL TVLHQDWLNG KEYKCKVSNK ALPAPIEKTI SKAKGQPREP	
8 351 QVYTLPPSRD ELTKNQVSLT CLVKGFYPSD IAVEWESNGQ PENNYKTTPP	
9 401 VLDSDGSFFL YSKLTVDKSR WQQGNVFSCS VMHEALHNHY TQKSLSLSPG	
10 451 K	
Upload Save Cancel	
	C



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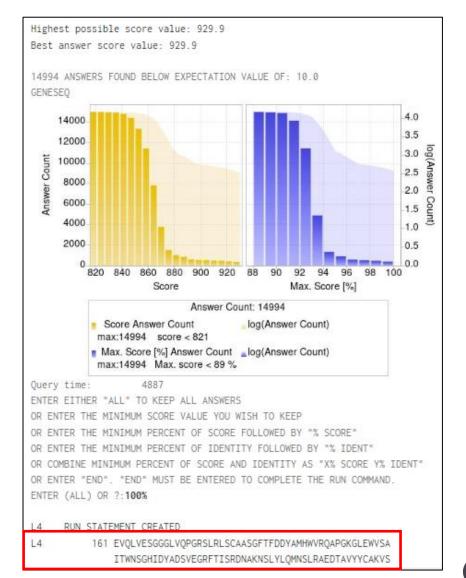
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GENESEQ BLAST search for Humira heavy chain

File GENESEQ
=>
Uploading sequence file: Humira heavy chain
UPLOAD SUCCESSFULLY COMPLETED L3 GENERATED
=> RUN BLAST L3/ SQP -F F
Algorithm: BLAST - BLASTP. Version: 2.12.0+



GENESEQ BLAST search for Humira heavy chain (cont.)



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Humira light chain

Edit Biosequence	×
Humira light chain Image: Check your sequence with the Validate button. Save As Image: Check your sequence with the Validate button. 1 DIQMTQSPSS LSASVGDRVT ITCRASQGIR NYLAWYQQKP GKAPKLLIYA 2 51 ASTLQSGVPS RFSGSGSGTD FTLTISSLQP EDVATYYCQR YNRAPYTFQQ 3 101 GTKVEIKRTV AAPSVFIFPP SDEQLKSGTA SVVCLLNNFY PREAKVQMKV 4 151 DNALQSGNSQ ESVTEQDSKD STYSLSSTLT LSKADYEKHK VYACEVTHQG 5 201 LSSPVTKSFN RGEC	Validation
Upload Save Cancel	





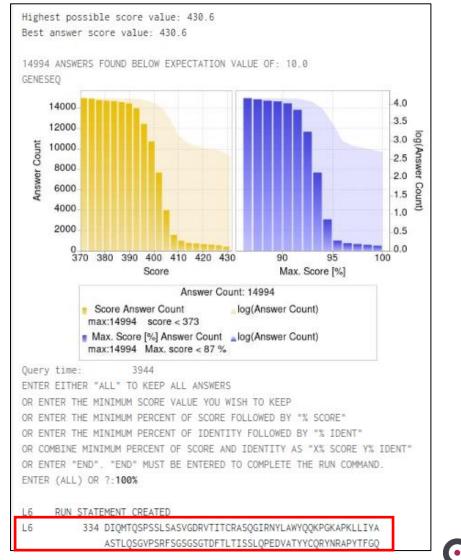


GENESEQ BLAST search for Humira light chain

File GENESEQ
=> Uploading sequence file: Humira light chain
UPLOAD SUCCESSFULLY COMPLETED L5 GENERATED
=> RUN BLAST L5/SQP -F F
Algorithm: BLAST - BLASTP. Version: 2.12.0+



GENESEQ BLAST search for Humira light chain (cont.)



CAS

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TRANSFER PNs into DWPI, AND sets together

=> FILE WPINDEX; TRA L4 PN 1-; TRA L6 PN 1-

L7 TRANSFER L4 1- PN : 110 TERMS L8 110 L7 ALL TERMS IN L7 RETRIEVED.	
L9 TRANSFER L6 1- PN : 233 TERMS L10 232 L9 ALL TERMS IN L9 RETRIEVED.	
=> S L8 AND L10	
L11 108 L8 AND L10	



Check DCR

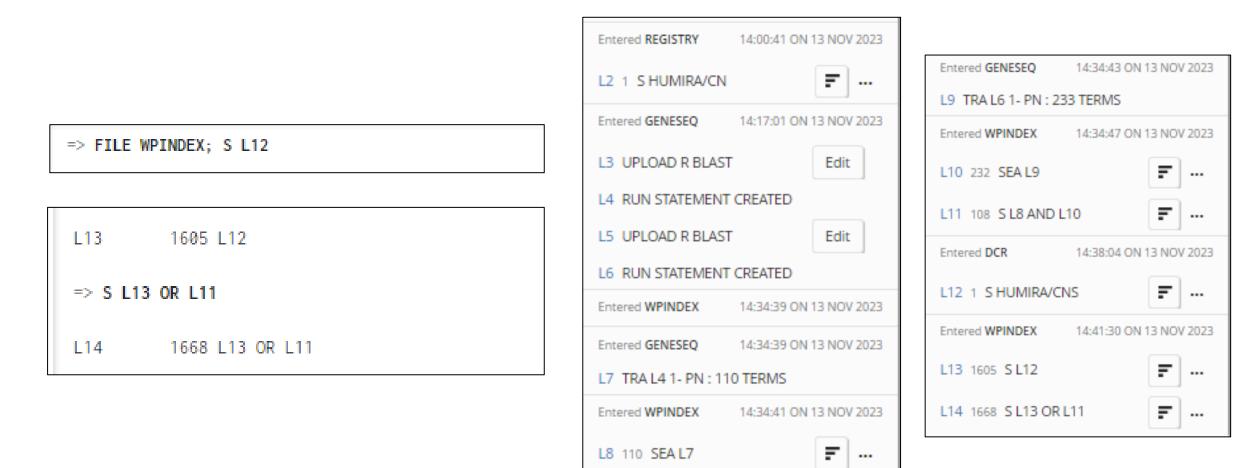
=> FILE DCR; S HUMIRA/CNS

L12	1 HUMIRA/CNS
=> D	
L12	ANSWER 1 OF 1 DCR COPYRIGHT 2023 CLARIVATE on STN.
AN	DCR-463982 DCR
	463982-0-0-0
CN.P SY	
STR	ADALIMUMAB; D-2-E-7; HUMIRA; TRUDEXA
	Substance image not available
CMT	An antibody of unknown structure.Immunoglobulin G1, anti-(human tumor
	necrosis factor)(human monoclonal D2E7 heavy chain), disulfide withhuman monoclonal D2E7 light chain, dimer.Molecular weight is approximately
	148,000 daltons
MF	Unknown
ED	Entered STN: 8 Aug 2003
	Last updated on STN: 1 Aug 2014
	Update DWPI Cross Ref.: 9 Nov 2023





Add that to DWPI search



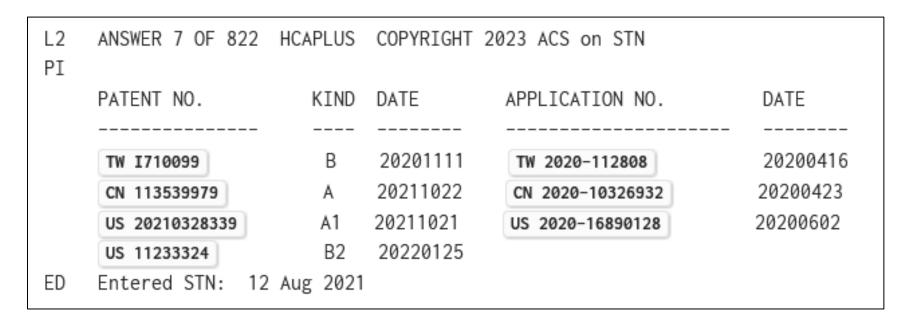


Dates to consider

- Date of publication is not the same as date of availability!
- Publication date vs. Entry date vs. Update date(s)
 - i.e., if record is retrieved by an index term, the update date of the indexing may become important



CAplus Publication Date vs. Entry Date



CAplus does not display Update Dates.



DWPI Publication Date vs. Entry Date

