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CWM Global Search

Finding unusual peptides on the Internet using plain three letter sequence codes.

Dr. Hans-Juergen Himmler, contact@hjhimmler.de , *Dr. Alexander Kos*, ***globalsearch@akosgmbh.de***, ***AKos*** *GmbH, Austr. 26, 79585 Steinen, Germany*

ECCB 2012 Basel, Tech Track session

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CWM Global Search

CWM Global Search provides a single User Interface that allow to perform a true federated search over all major free accessible chemistry databases and drug discovery data sources on the Internet using

- Chemical structure
- Chemical name
- CAS Registry numbers

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Major characteristics of CWM Global Search :

- As easy to use as Google (Single structure box, single text box and one button to start the search)
- Other than Google only science relevant data sources are searched
- Like in Google the result of the search are links
- Unlike Google result links can be sorted, filtered and grouped
- Allows search for multiple independent search terms with one single click
- Queries are automatically extended if possible

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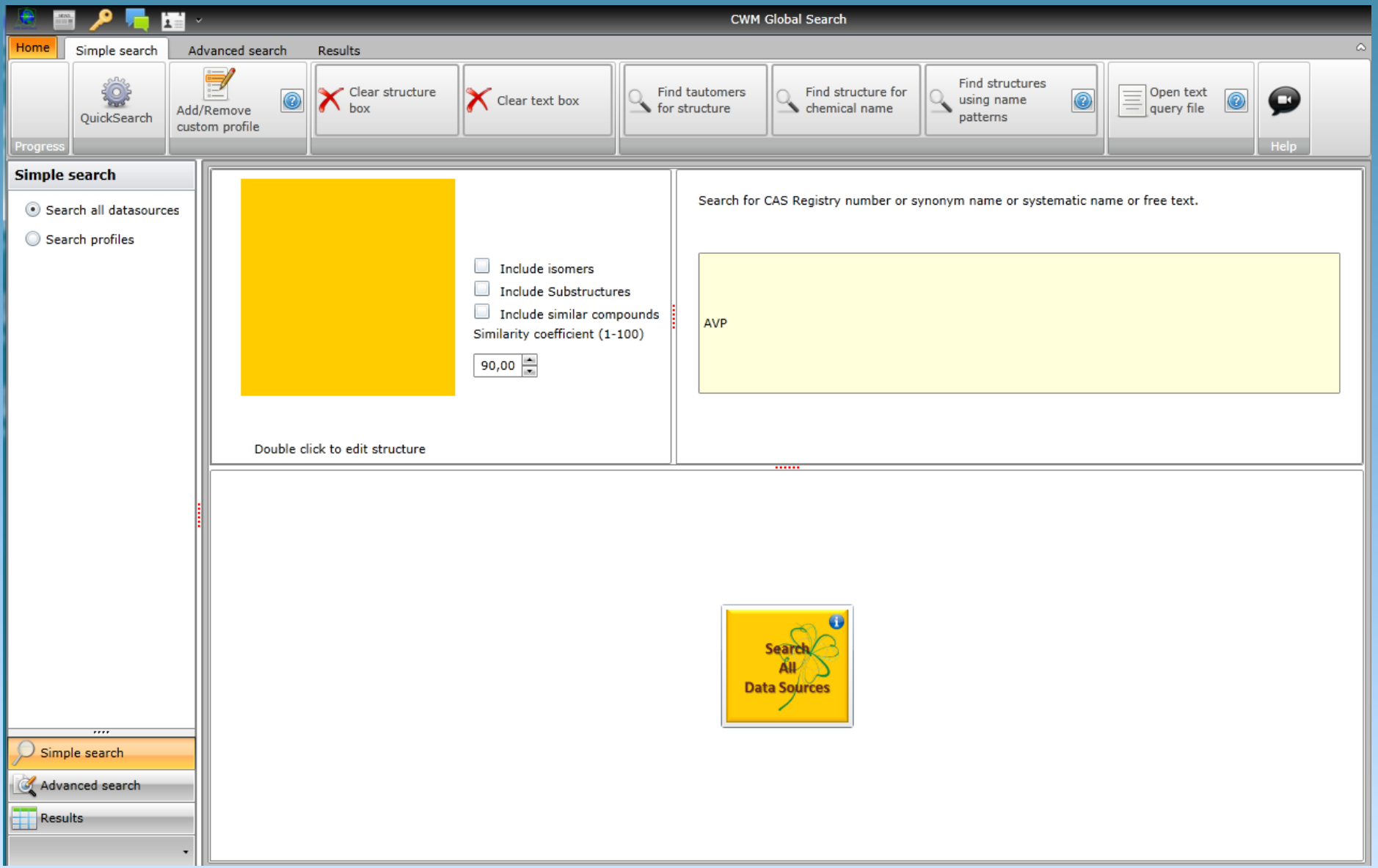

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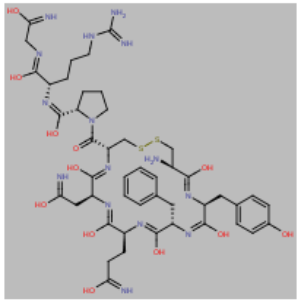
Home | Simple search | Advanced search | Results

Results

Structure

Double click to zoom structure



Globalsearch links | Quicklinks

Remove all filter

RECORD_1 27

1 2

Drag a column header and drop it here to group by that column

Ra		Datasource	Link	Category	Keywords	Searchtype	Query
1		PubChem	Hit(s) found	Bioactivity		SYNONYMNAME	"Arginine antidiuretic hormone"
1		PubChem	Hit(s) found	Bioactivity		SYNONYMNAME	Rindervasopressin
11		ChEBI	100 ChEBI ID(s) found.	Bioactivity		SYNONYMNAME	"Arginine antidiuretic hormone"
1		PubChem	Hit(s) found	Bioactivity		FULLSTRUCTURE	
63		EBI	Total hit(s) 0	Bioactivity		SYNONYMNAME	"Arginine antidiuretic hormone"
47		ChEMBL	CHEMBL373742	Bioactivity		FULLSTRUCTURE	
60		ChemBank	CHEMBANK ID found	Bioactivity		MOLSIMILARITY	
6		Chemicalland21	2 Hit(s)	Chemistry		SYNONYMNAME	"Arginine antidiuretic hormone"
2		ChemSpider	Hit(s) found	Chemistry		SYNONYMNAME	"Arginine antidiuretic hormone"
2		ChemSpider	Hit(s) found	Chemistry		SYNONYMNAME	Rindervasopressin
2		ChemSpider	Hit(s) found	Chemistry		FULLSTRUCTURE	
2		ChemSpider	Hit(s) found	Chemistry		FULLSTRUCTURE	
37		NextBio	PubChem Substance NextBio link foun	Drugs		FULLSTRUCTURE	
10		Quertle	(35) relationships	Literature		SYNONYMNAME	"Arginine antidiuretic hormone"
31		Google Books	Books 1 - 10 of 10	Literature		SYNONYMNAME	"Arginine antidiuretic hormone"
31		Google Books	Books 1 - 10 of 23	Literature		SYNONYMNAME	Rindervasopressin
33		PubMed	Results: 2	Literature		SYNONYMNAME	"Arginine antidiuretic hormone"
41		PubMedCentral	Results: 1 to 20 of 1822	Literature		SYNONYMNAME	"Arginine antidiuretic hormone"
41		PubMedCentral	Results: 4	Literature		SYNONYMNAME	Rindervasopressin

Simple

Advan

Result

Right click for menu

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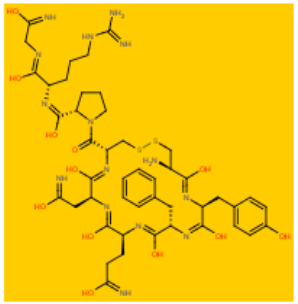
Home | Simple search | Advanced search | Results

Advanced search

9/7/2012 12:56:22 PM
9/7/2012 1:00:12 PM
Read only query page

Simple search
Advanced search
Results

Double click to edit structure



Structure Search
- [ ] Include isomers
- [ ] Include Substructures
- [ ] Include similar compounds

Similarity coefficient (1-100) 90,00

Use the rightmost 'Pin' button to show/hide this pane

Free text

07.09.2012 13:00:12

1

Free text
Click here to add new item
[8-Arginine]vasopressin
[Arg8]-Vasopressin
"1,2-Dithia-5,8,11,14,17-pentaazacycloeicosane-10-propi
3-(Phenylalanine)-8-arginineoxytocin
8-L-Arginine-vasopressin
Arg8-vasopressin
☑ "Arginine antidiuretic hormone"
Arginine-8-vasopressin
Arginine-vasopressin
"Cys-Tyr-Phe-Gln-Asn-Cys-Pro-Arg-Gly-NH2[Disulfide Brid
"Glycinamide, L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-gluta
NCGC00166306-01
"Oxytocin, 3-(L-phenylalanine)-8-L-arginine-"
☑ Rindervasopressin
"roxybenzyl-6,9,12,15,18-pentaoxo- (6CI)"
"Vasopressin, 8-L-arginine- (7CI,8CI,9CI)"
(2S)-2-{[(2S)-1-[(4R,7S,10S,13S,16S,19R)-19-amino-13

Use the rightmost 'Pin' button to show/hide this pane

Filter | Remove all filter
Filter operations

07.09.2012 13:00:12

1 2 3 4

Drag a column header and drop it here to group by that column

Rank		Name
40	☑	ACS Publications
5	☑	AKOSSAMPLES
40	☑	Bielefeld Academic Search Engine
42	☑	BindingDB
25	☑	BioMed Central
61	☑	BMRB
15	☑	Buyersguide
26	☑	CCRIS
11	☑	ChEBI
24	☑	ChemAxon Chemicalize Search
60	☑	ChemBank
47	☑	ChEMBL
62	☑	Chemeo
7	☑	ChemExper
4	☑	ChemicalBook
18	☑	CHEMICALDATABASE
6	☑	Chemicalland21
27	☑	ChemIDPlus
2	☑	ChemSpider
21	☑	ChemSynthesis

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Finding unusual peptides on the Internet using plain three letter sequence codes.

Scenario 1

The Effects of N-Terminal Part Modification of Arginine Vasopressin Analogues with 2-Aminoindane-2-carboxylic Acid: A Highly Potent V_2 Agonist

Wioleta Kowalczyk,*,† Dariusz Sobolewski,† Adam Prahl,† Izabela Derdowska,† Lenka Borovičková,‡ Jiřina Slaninová,‡ and Bernard Lammek†

Faculty of Chemistry, University of Gdańsk, Sobieskiego 18, 80-952 Gdańsk, Poland, and Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Flemingovo sq. 2, 16610 Prague, Czech Republic

Received February 15, 2007

In this study we present the synthesis and some pharmacological properties of nine new analogues of arginine vasopressin modified in the N-terminal part of the molecule with 2-aminoindane-2-carboxylic acid (Aic). The peptides were tested for their in vitro uterotonic and in vivo pressor and antidiuretic activities. One of the new peptides, [Mpa^1,Aic^2,Val^4,D-Arg^8]VP, exhibited an antidiuretic activity similar to that of [Mpa^1,D-Arg^8]VP, thus being one of the most potent antidiuretic vasopressin analogues reported to date.

Introduction

Arginine vasopressin (AVP[a]), a neuropeptide, exerts its action through at least three types of G-protein-coupled receptors with seven transmembrane spanning domains. V_1 vascular receptors

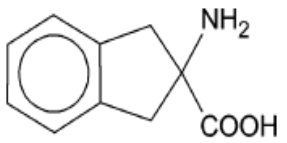

Figure 1. Structure of 2-aminoindane-2-carboxylic acid (Aic).

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The task:

How do I find Arginine Vasopressin analogues with unusual amino acid residues in position 2 of AVP that show antidiuretic activity ?

A possible approach :

Search through the ChEBI database, since this database contains biological active peptides with associated assay results

The problem :

In the ChEBI database you can not do BLAST searches such as Cys-X-Phe-Gln-Asn-Cys-Pro-Arg-Gly instead you need to perform a structure search

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The solution:

CWM Global Search professional with Proteax option !

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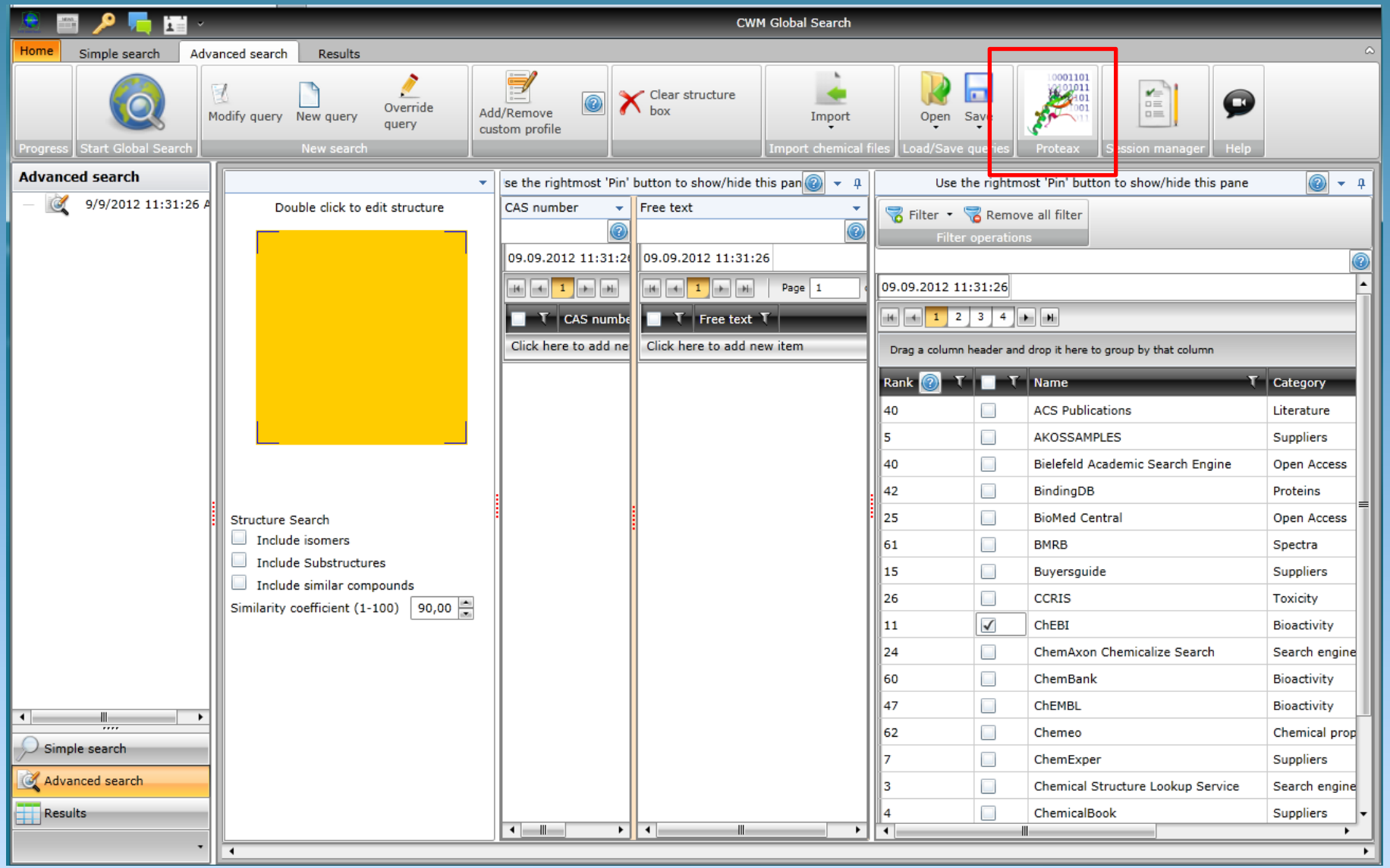

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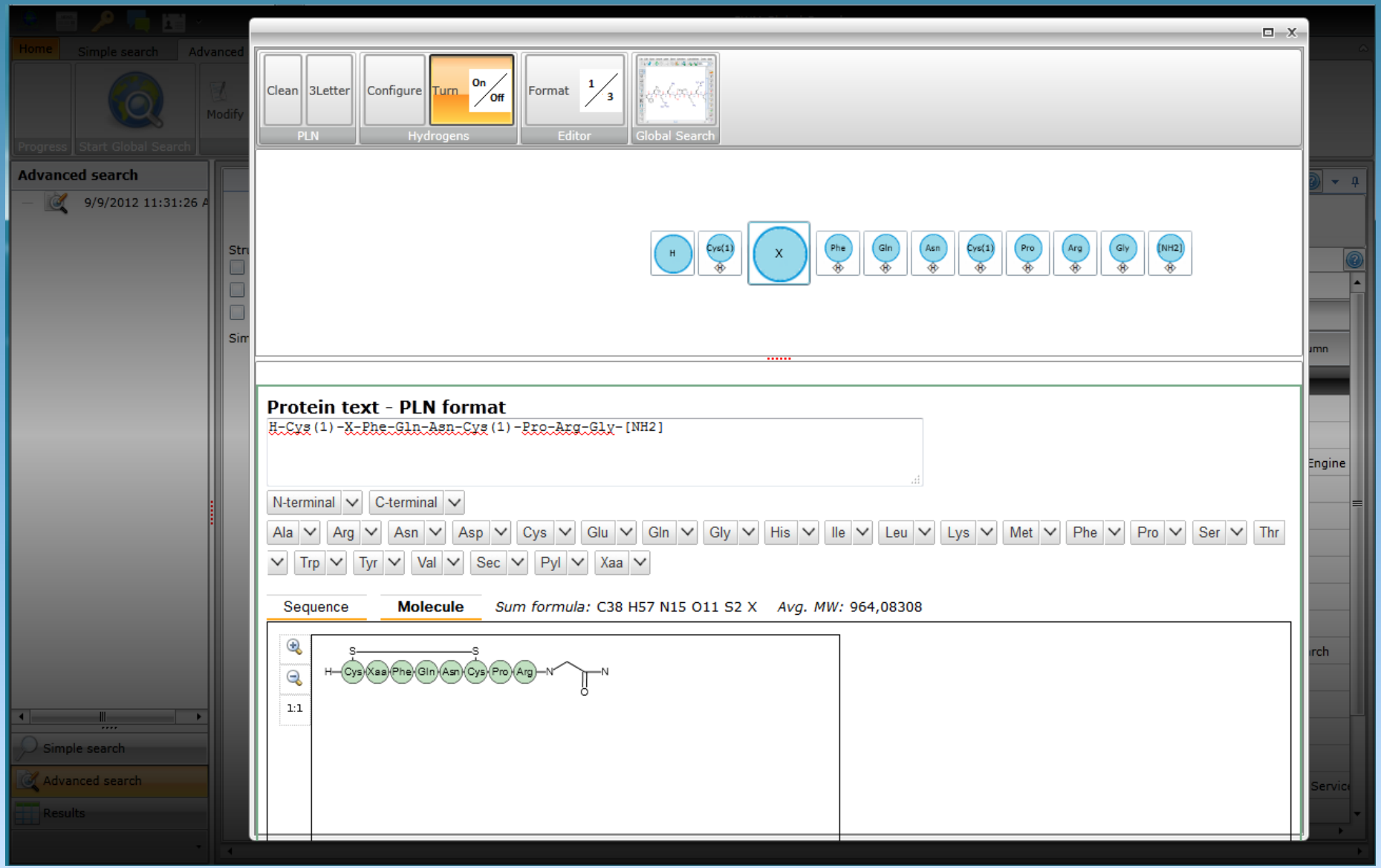

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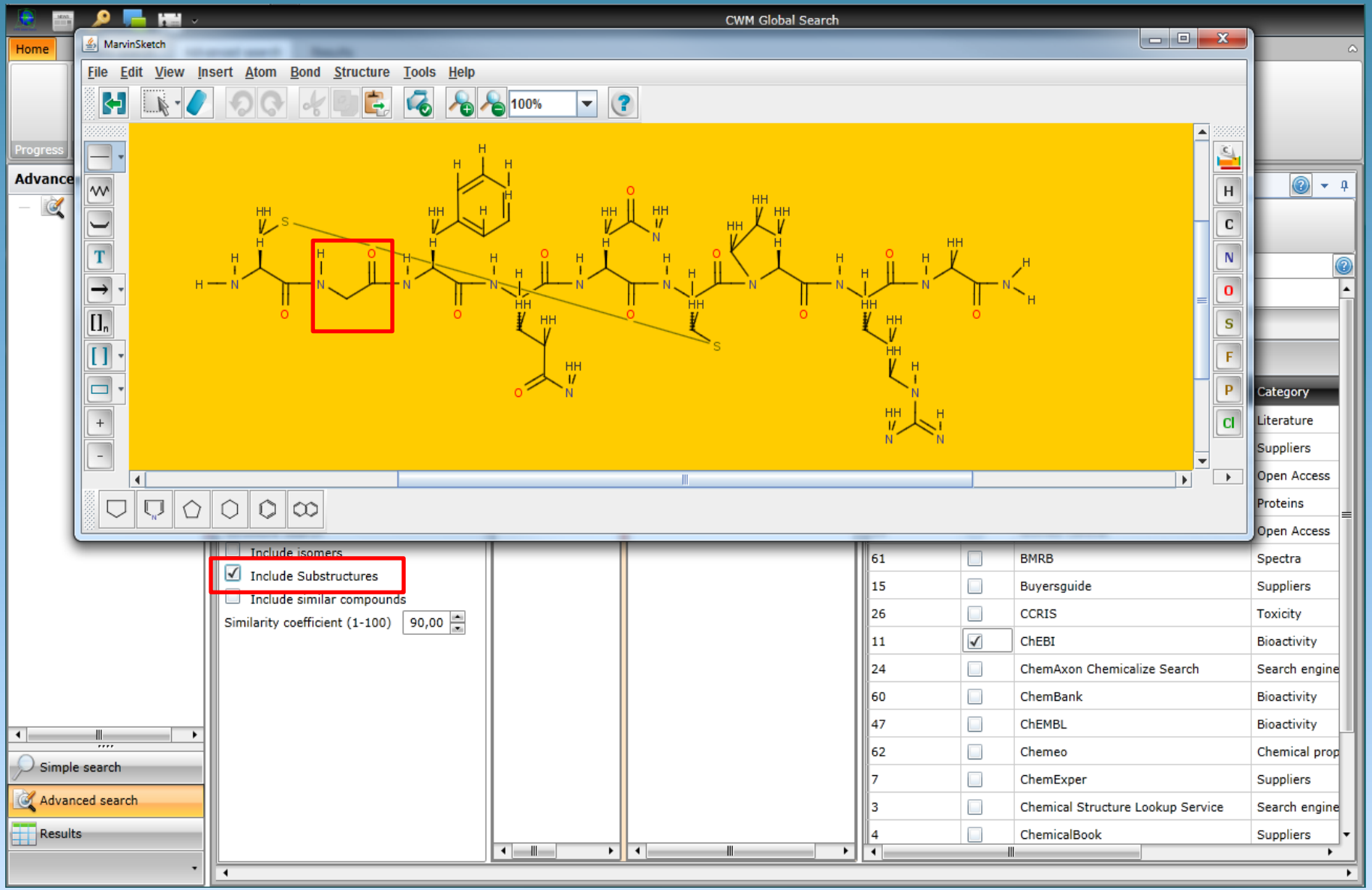

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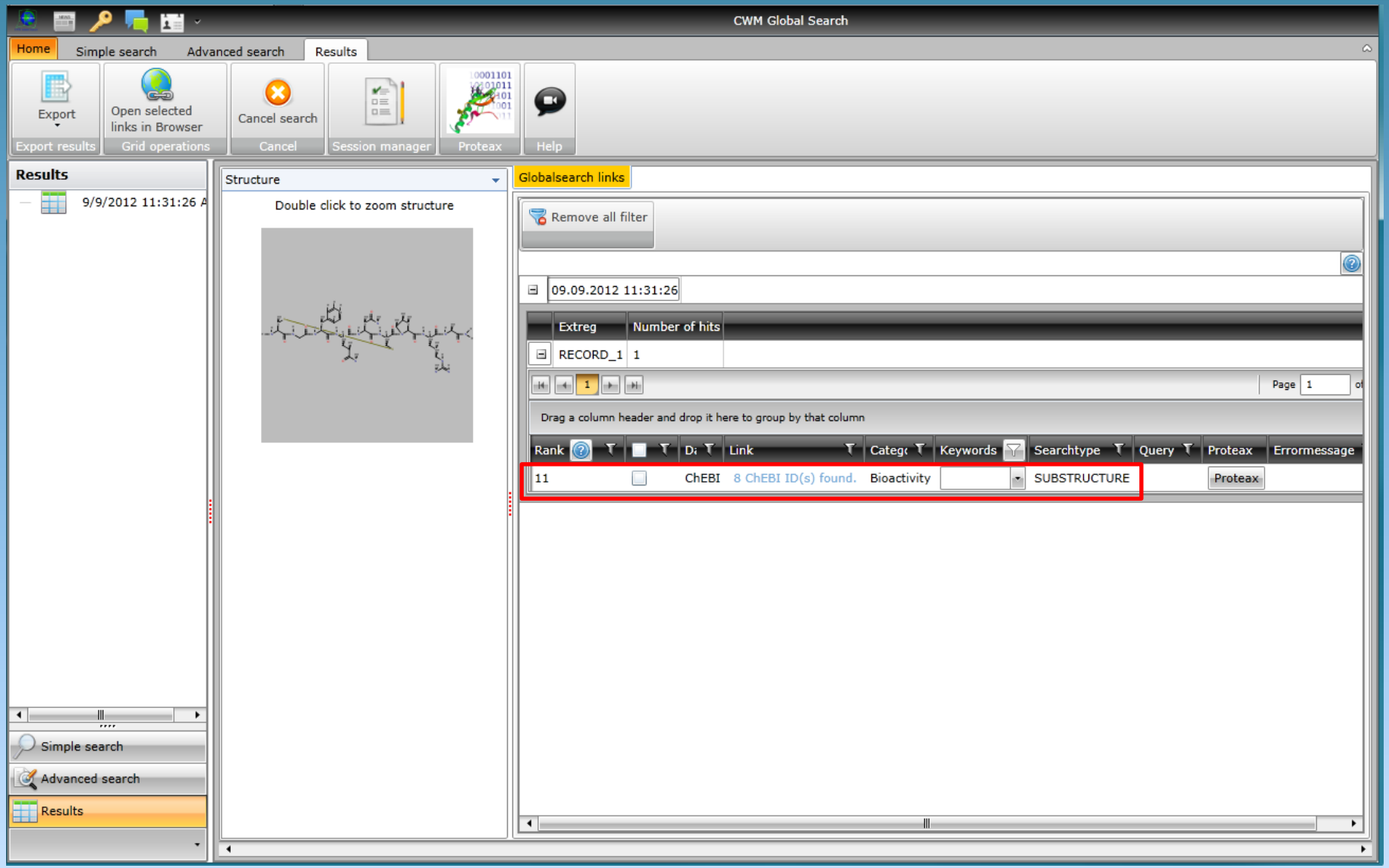

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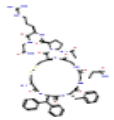
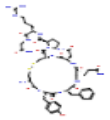
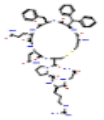
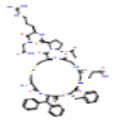
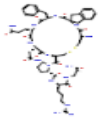
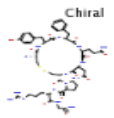
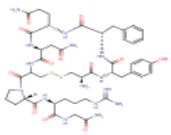
Another problem :

Peptides in ChEBI are not represented in 3 or 1 letter sequence codes and therefore make the intepretation of the results rather difficult

The results in ChEBI :

8 entries found, displaying 1 to 8. << < 1 > >>

 CHEBI:655167 (ChEMBL) (S)-N-((R)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,16R,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-16-benzhydryl-13-benzyl-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carbonyl)pyrrolidine-2-carboxamide	 CHEBI:655164 (ChEMBL) (S)-N-((R)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,16S,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13-benzyl-16-(4-hydroxybenzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carbonyl)pyrrolidine-2-carboxamide	 CHEBI:658626 (ChEMBL) (S)-N-((R)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,16S,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-16-benzhydryl-13-benzyl-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carbonyl)pyrrolidine-2-carboxamide
 CHEBI:656873 (ChEMBL) (S)-N-((S)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,16R,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-16-benzhydryl-13-benzyl-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carbonyl)pyrrolidine-2-carboxamide	 CHEBI:1271649 (ChEMBL) (S)-N-((S)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,16S,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13,16-dibenzyl-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosane-4-carbonyl)pyrrolidine-2-carboxamide	 CHEBI:658624 (ChEMBL) (S)-N-((S)-1-(2-amino-2-oxoethylamino)-5-guanidino-1-oxopentan-2-yl)-1-((4R,7S,10S,13S,19R)-19-amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13-benzyl-6,9,12,15,18-pentaoxo-1',3'-dihydro-1,2-dithia-5,8,11,14,17-pentaazaspiro[[1,2]cycloicosane-16,2'-indene]-4-ylcarbonyl)pyrrolidine-2-carboxamide
 CHEBI:466860 (ChEMBL) CHEBI:466860	 CHEBI:34543 argipressin Stars: ★★★	

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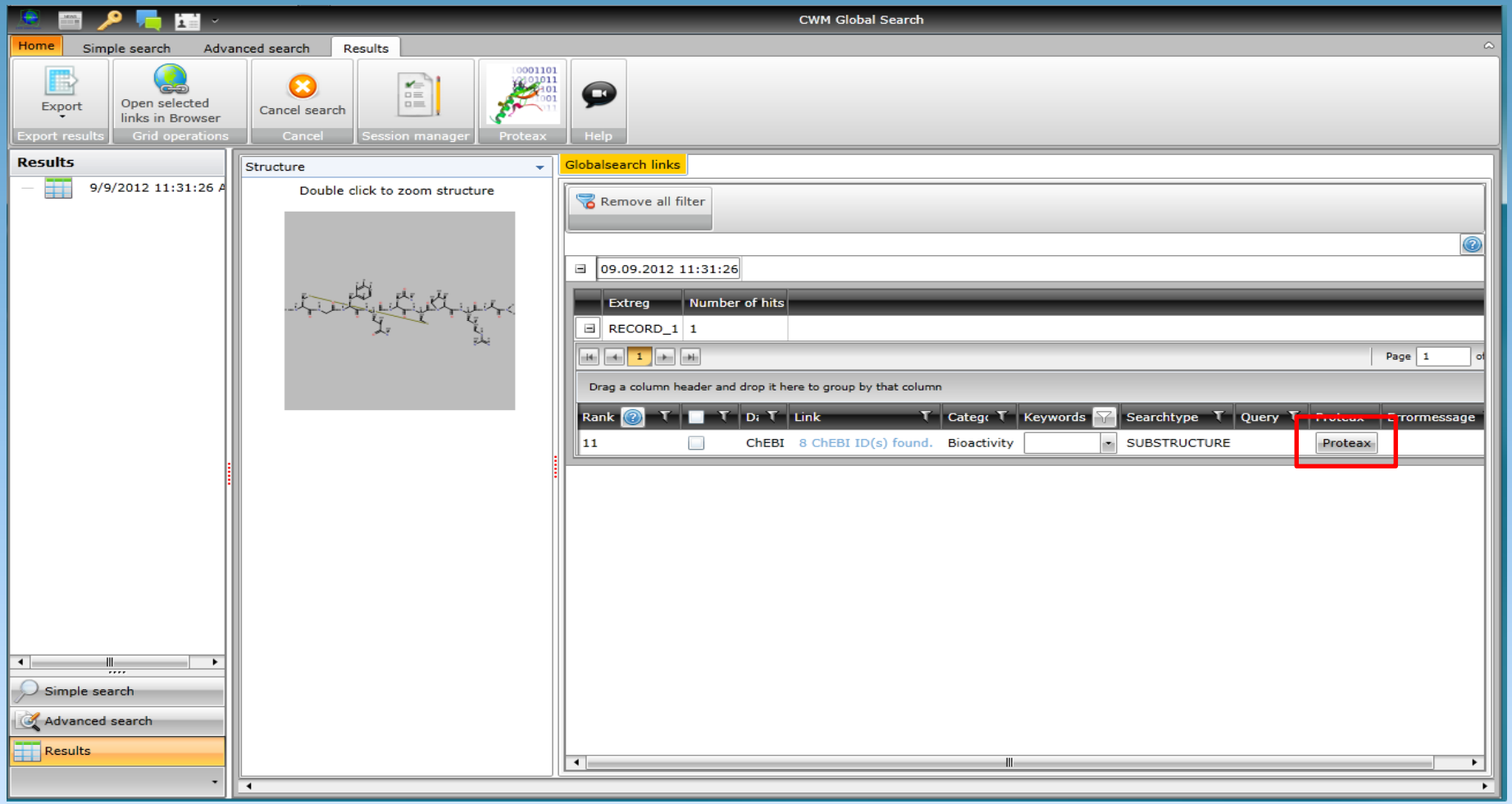
The solution :

The structure -> 1(3) letter sequence code converter in Proteax



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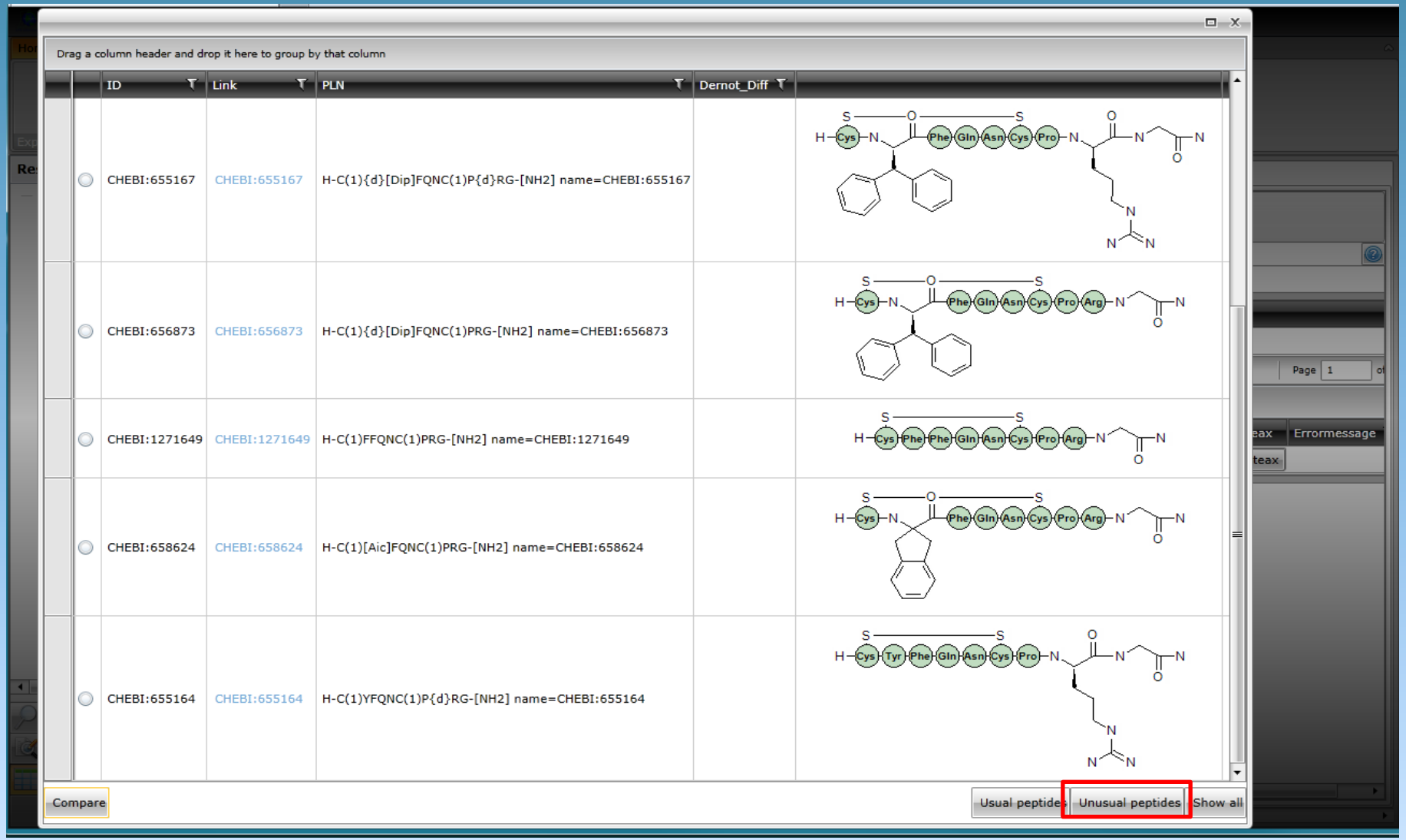
The same ChEBI result in CWM Global Search with integrated Proteax



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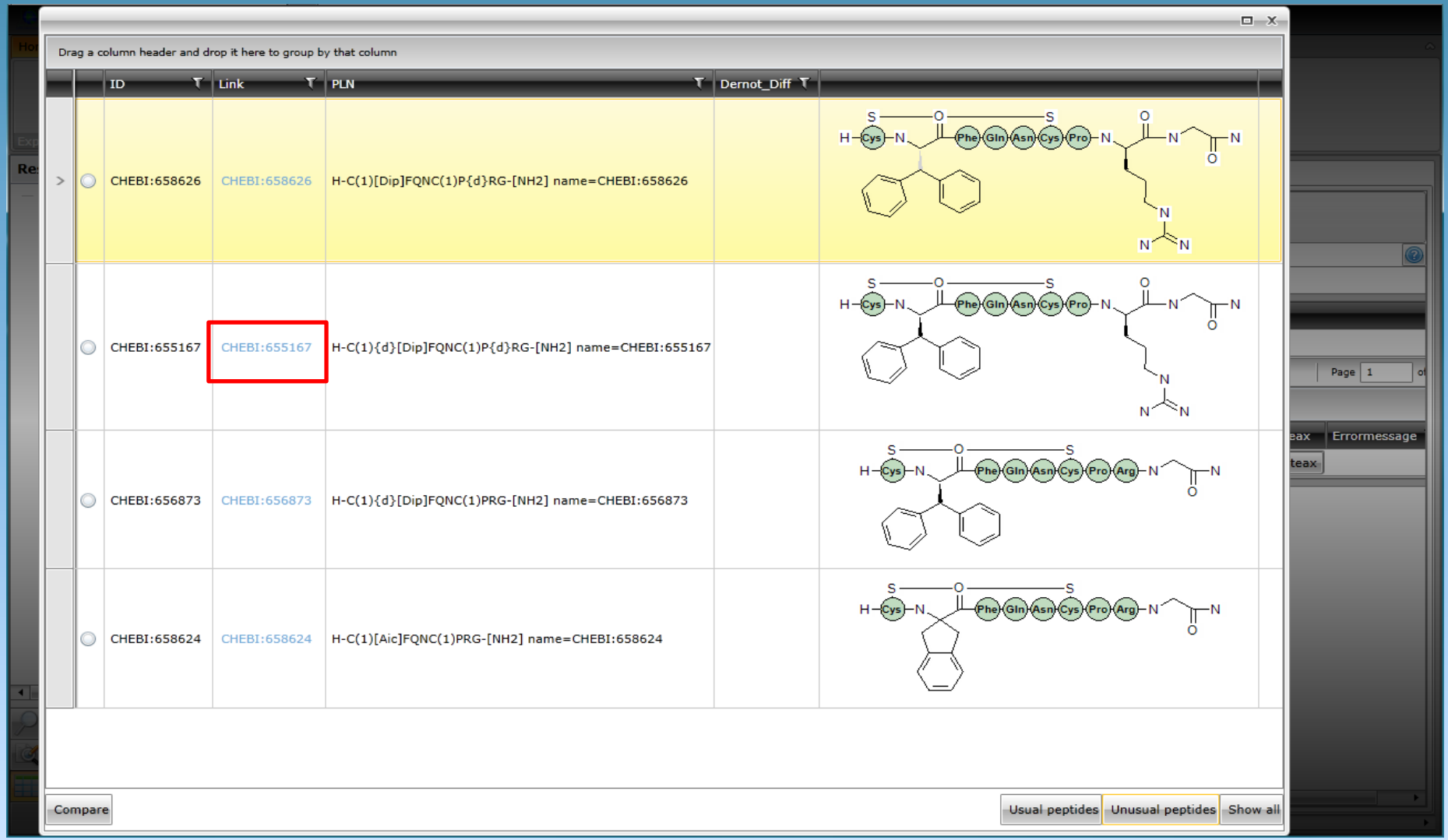
Show only ‚unusual' peptides and open ChEBI record for specific peptide



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ChEMBL

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- ChEMBL-NTD
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- GPCR SARfari
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- ChEMBL Group
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ChEMBLdb Statistics

- DB: ChEMBL_14
- Targets: 9,003
- Compound records: 1,376,469
- Distinct compounds: 1,213,239
- Activities: 10,129,256
- Publications: 46,133

ChEMBL Blog

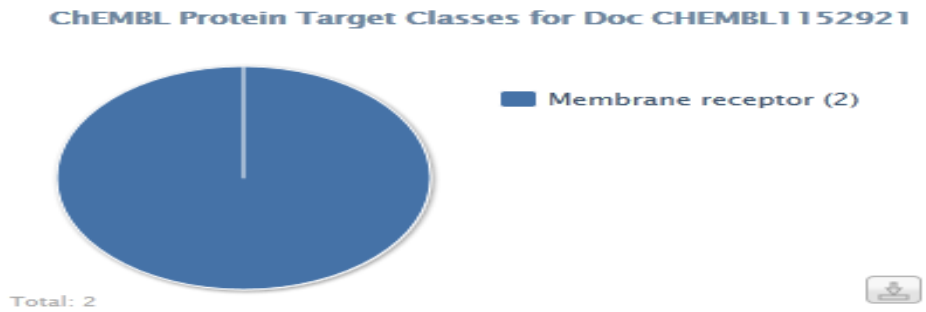
- New Drug Approvals 2012 - Pt. XVII - Linaclotide (LinzessTM)
- Antibody Drugs To Have Reached Clinical

EBI > Databases > Small Molecules > ChEMBL Database

Document Report Card

Doc ID	CHEMBL1152921
Journal	Eur. J. Med. Chem. (2009) 44:2862-2867
Title	Arginine vasopressin and its analogues--the influence of position 2 modification with 3,3-diphenylalanine enantiomers. Highly potent V2 agonists.
Authors	Kwiatkowska A, Sobolewski D, Prahl A, Borovickova L, Slaninova J, Lammek B
Abstract	Eleven new analogues of arginine vasopressin (AVP) modified in position 2 by 3,3-diphenyl-L-alanine or its D-enantiomer (Dip or D-Dip) were synthesized and pharmacologically evaluated for their pressor, antidiuretic and in vitro uterotonic activities. Both the Dip and D-Dip modifications at position 2 of AVP are sufficient to completely change the pharmacological profile of the peptides. They preserve or increase antidiuretic activity, cause its prolongation, transform uterotonic property in antagonistic one and cancel the effect on blood pressure. Four of the new peptides ([Mpa1,D-Dip2]AVP, [Mpa1,D-Dip2,Val4]AVP, [Mpa1,D-Dip2,D-Arg8]VP, [Mpa1,D-Dip2,Val4,D-Arg8]VP) are exceptionally potent antidiuretic agents with significantly prolonged activities.
CiteXplore	19418631
DOI	

Protein Target Summary



Assay Summary

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Finding unusual peptides on the Internet using plain three letter sequence codes.

Scenario 2

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The task:

How do I find specifically NON CYCLIC nona peptides with two cysteine residues in position 1 and 6 in the ChEBI database and in PubChem ?

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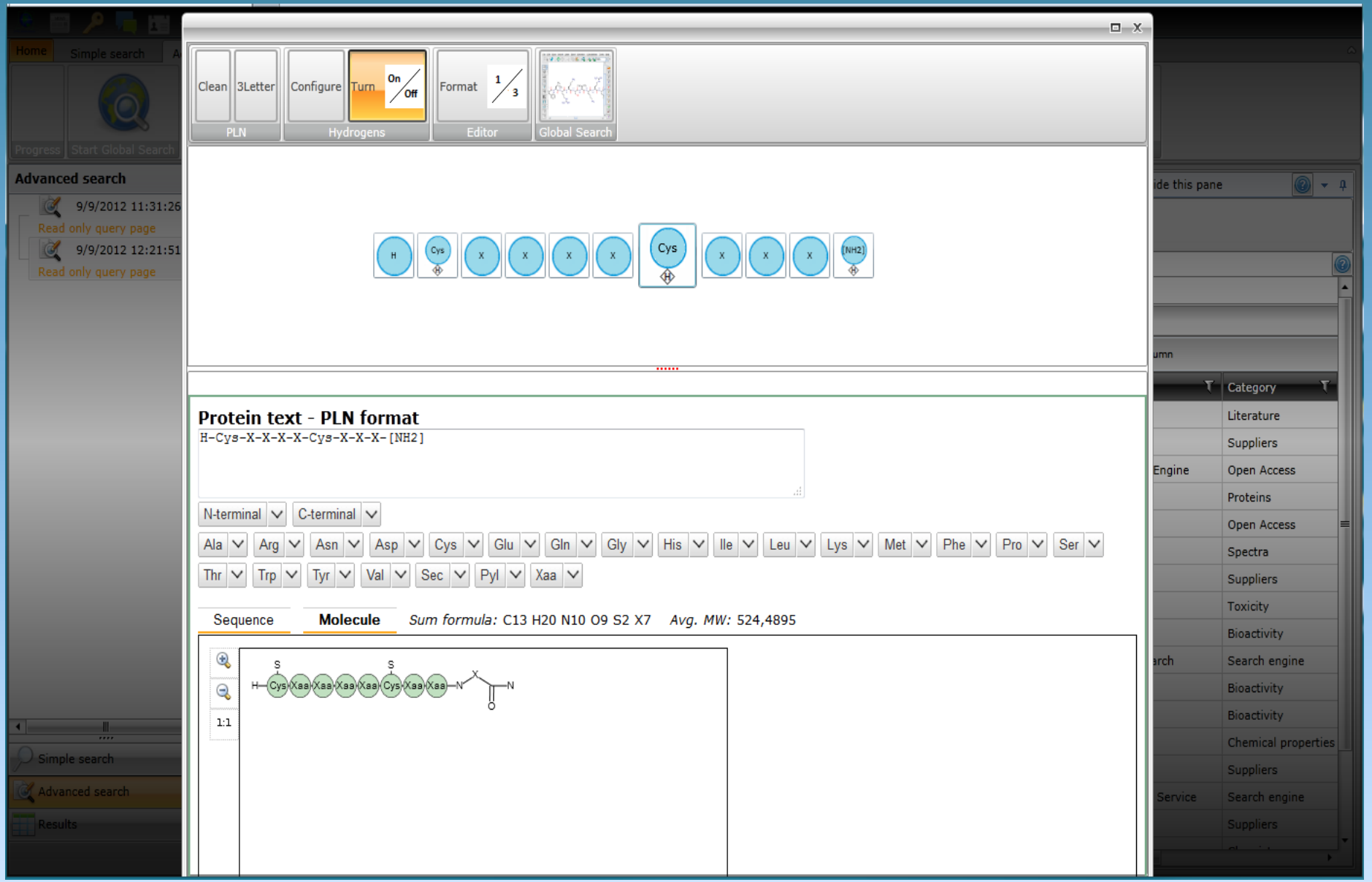

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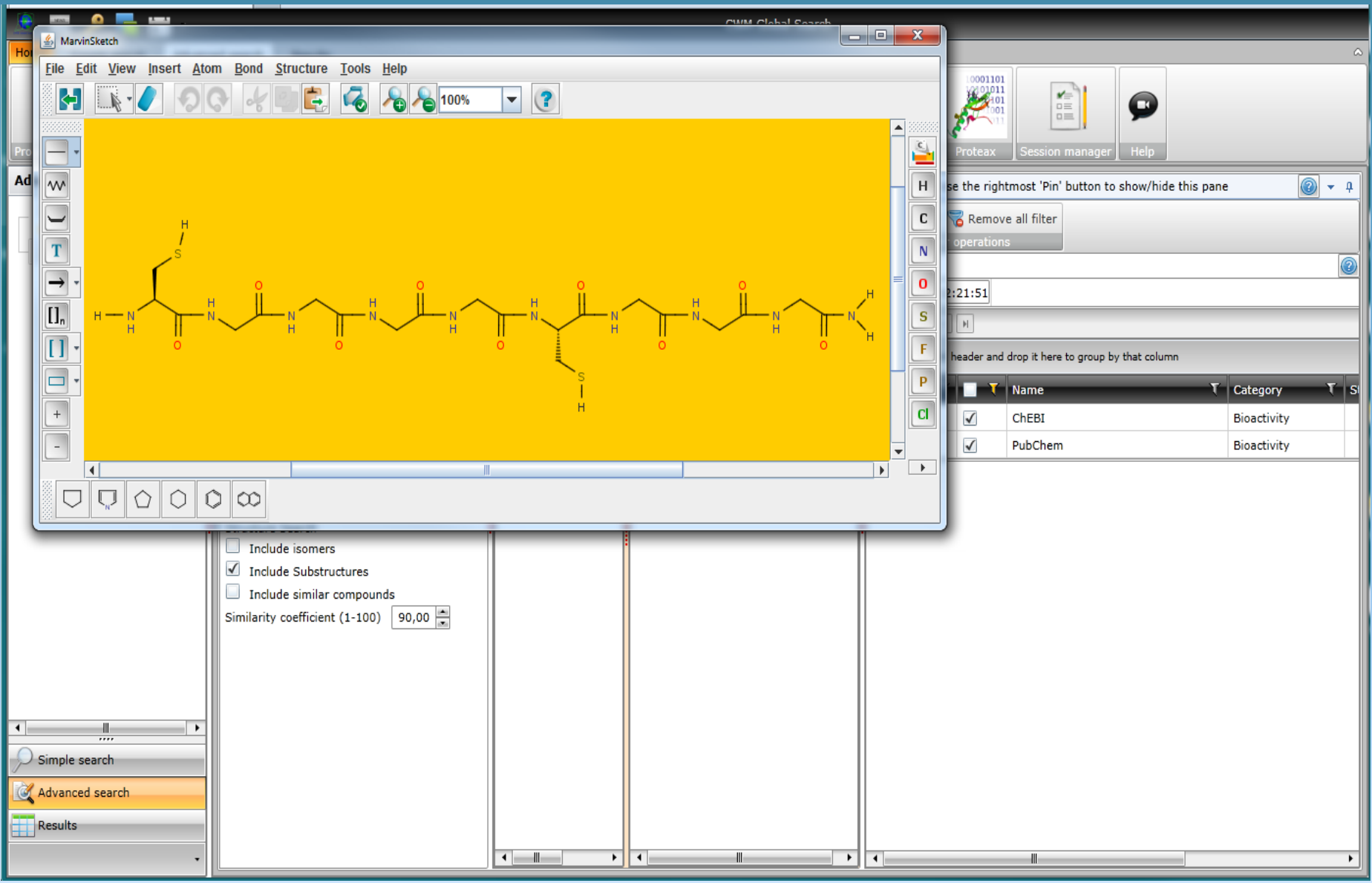

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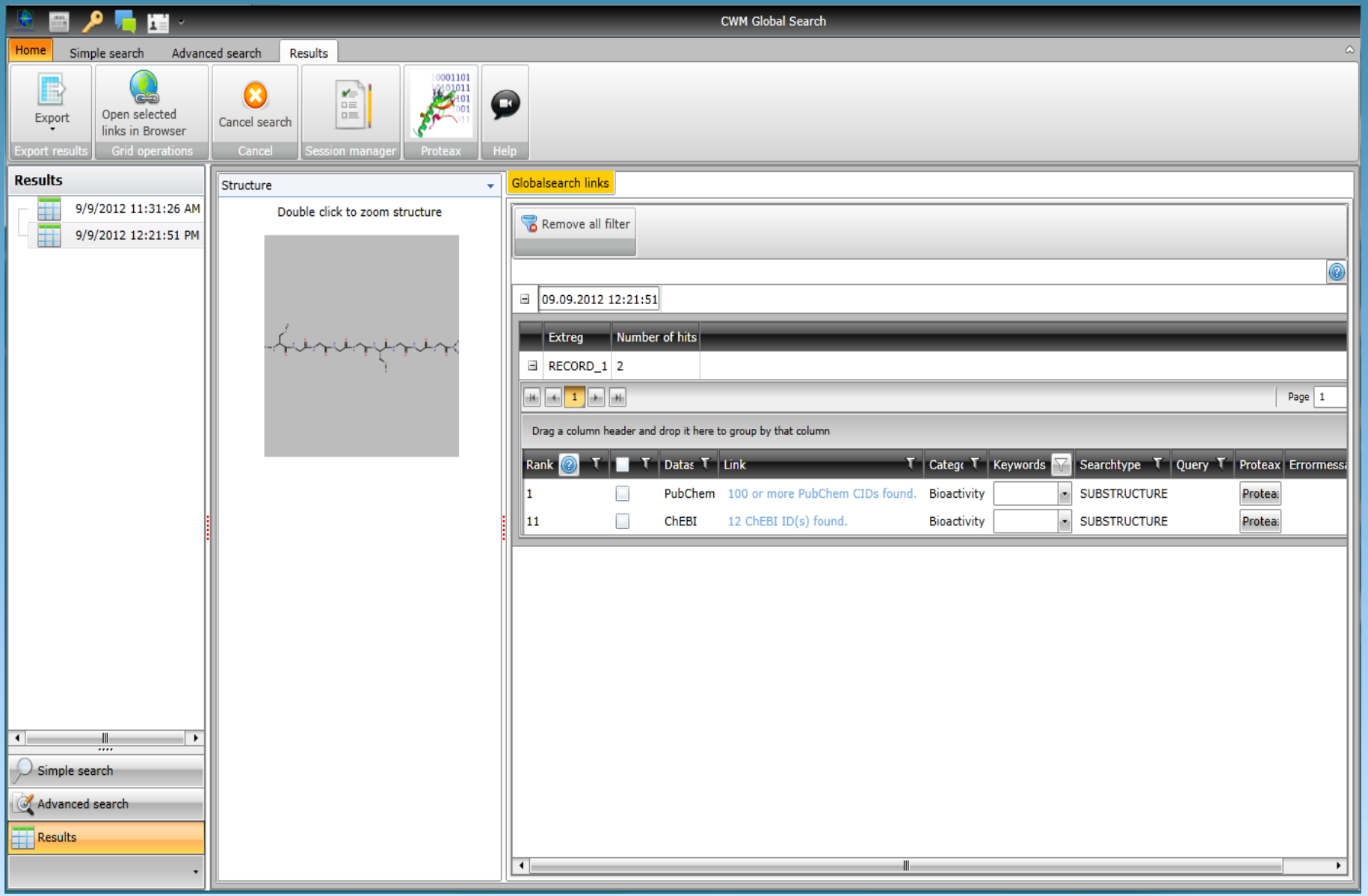

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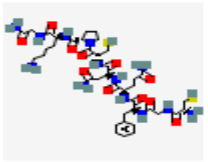
The result in the PubChem database

5. 
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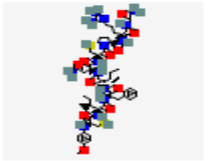
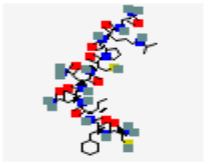
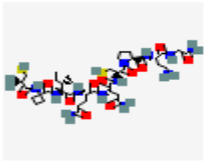
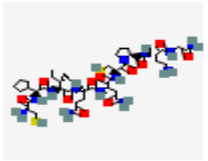
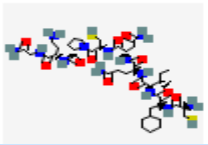
IUPAC name: (2S)-N-[(2S)-4-amino-1-[[(2R)-1-[(2S)-2-[[(2S)-6-amino-1-[(2...
CID: **42641084**
Similar Compounds

6. 
MW: 1127.382220 g/mol MF: $C_{51}H_{78}N_{14}O_{11}S_2$
IUPAC name: (2S)-N-[(2R)-1-[(2S)-2-[[(2S)-1-[(2-amino-2-oxoethyl)amino]-...
CID: **42640861**
Similar Compounds

7. 
MW: 1028.292680 g/mol MF: $C_{44}H_{77}N_{13}O_{11}S_2$
IUPAC name: (2S)-2-[[(2S)-4-amino-2-[[(2S,3S)-2-[[(2S)-2-[[(2R)-2-amino-...
CID: **24875712**
Similar Compounds

8. 
MW: 930.106620 g/mol MF: $C_{37}H_{63}N_{13}O_{11}S_2$
IUPAC name: (2S)-N-[(2S)-4-amino-1-[[(2R)-1-[(2S)-2-[[(2S)-4-amino-1-[(2...
CID: **24875711**
Similar Compounds

9. 
MW: 958.159780 g/mol MF: $C_{39}H_{67}N_{13}O_{11}S_2$
IUPAC name: (2S)-N-[(2S)-4-amino-1-[[(2R)-1-[(2S)-2-[[(2S)-4-amino-1-[(2...
CID: **24875625**
Similar Compounds

10. 
MW: 986.212940 g/mol MF: $C_{41}H_{71}N_{13}O_{11}S_2$
IUPAC name: (2S)-N-[(2S)-4-amino-1-[[(2R)-1-[(2S)-2-[[(2S)-4-amino-1-[(2...
CID: **24875624**
Similar Compounds

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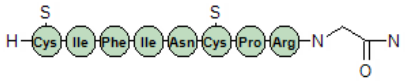
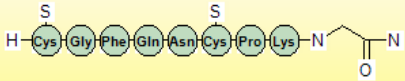
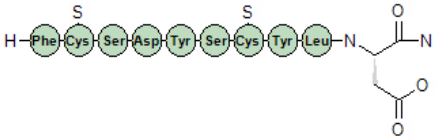
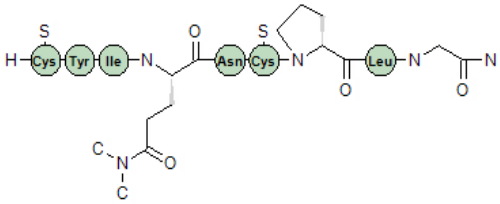
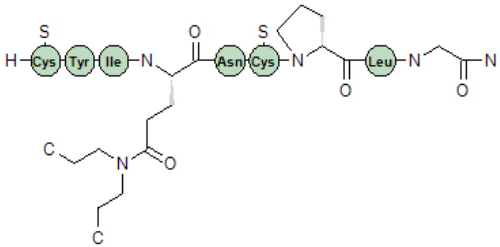
The result in CWM Global Search

Drag a column header and drop it here to group by that column

	ID	Link	PLN	Dernot_Diff	
○	42640861	42640861	H-CIFINCPRG-[NH2] name=42640861		
○	42641084	42641084	H-CGFQNCPKG-[NH2] name=42641084		
○	44277798	44277798	H-FCSDYSCYLD-[NH2] name=44277798		
○	44308796	44308796	H-CYI{d}[Glu[N(CH3)2]]NC{d}PLG-[NH2] name=44308796		
○	44308989	44308989	H-CYI{d}[Glu[N(nC3H7)2]]NC{d}PLG-[NH2] name=44308989		

Compare

Usual peptides | Unusual peptides | Show all

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Scenario 3 :

I have a PubChem hit list containing both small molecules and peptides and I only want to look at peptides and compare them !

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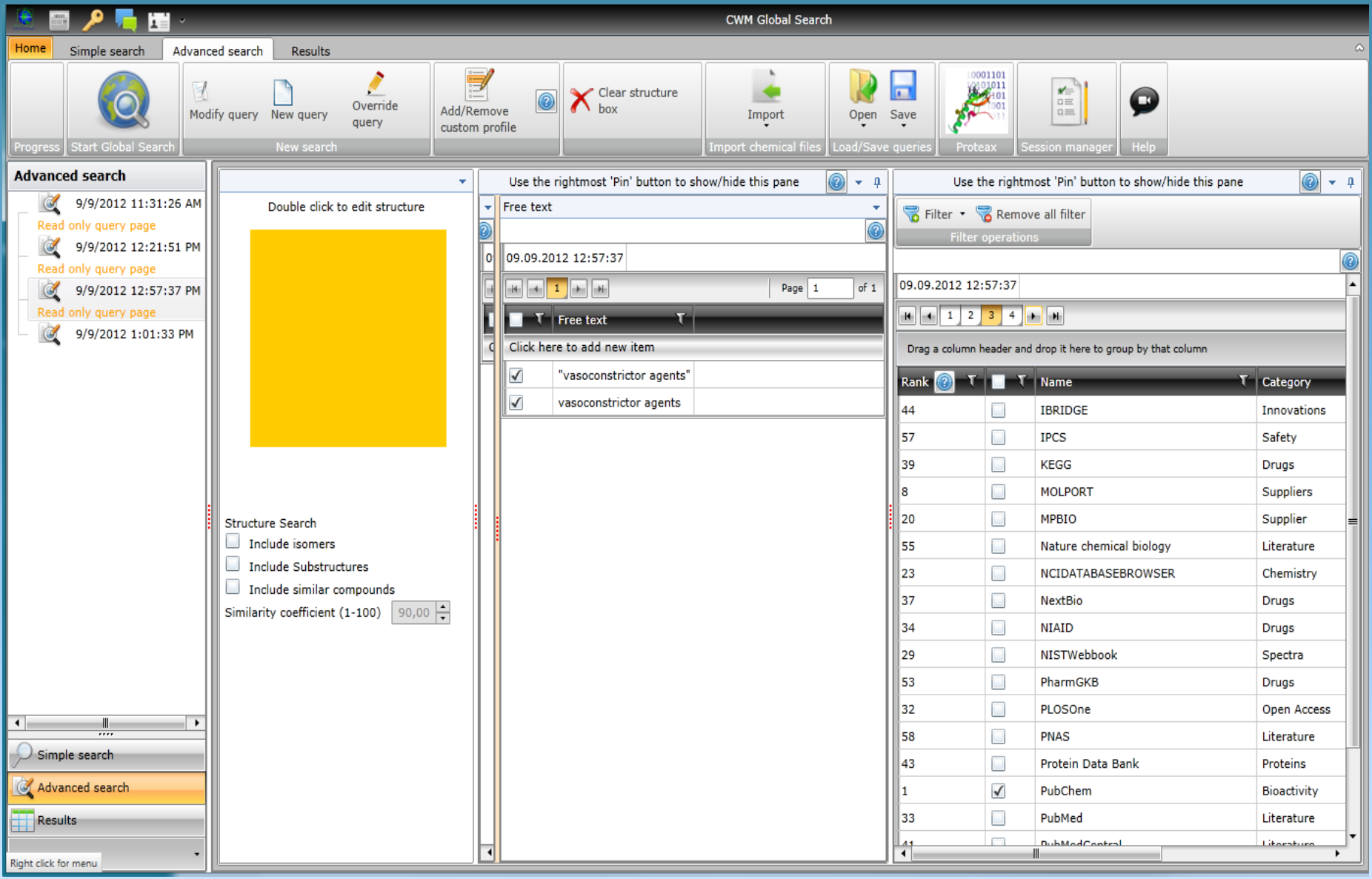

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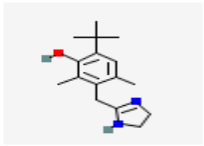
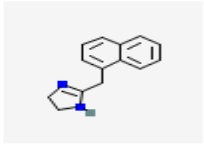
The result list in PubChem

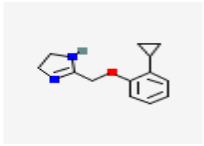
Results: 21 to 40 of 166

21. 

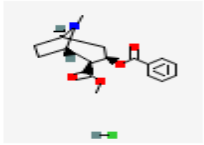
oxymetazoline; Oxymethazoline; Oxylazine ...
MW: 260.374560 g/mol MF: $C_{16}H_{24}N_2O$
IUPAC name: 6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dime...
Active in 44 BioAssays | Tested in 277 BioAssays
CID: 4636
Similar Compounds | Same Parent, Connectivity | Mixture/Component Compounds | BioAssays, activity ≤ 1 µM | PubMed (MeSH Keyword)

22. 

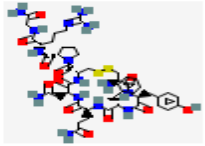
naphazoline; Naphthizine; Clearine ...
MW: 210.274360 g/mol MF: $C_{14}H_{14}N_2$
IUPAC name: 2-(naphthalen-1-ylmethyl)-4,5-dihydro-1H-imidazole
Active in 8 BioAssays | Tested in 144 BioAssays
CID: 4436
Similar Compounds | Same Parent, Connectivity | Mixture/Component Compounds | BioAssays, activity ≤ 1 µM | PubMed (MeSH Keyword)

23. 

cirazoline; Cirazolinum [INN-Latin]; Cirazolina [INN-Spanish] ...
MW: 216.278940 g/mol MF: $C_{13}H_{16}N_2O$
IUPAC name: 2-[(2-cyclopropylphenoxy)methyl]-4,5-dihydro-1H-imidazole
Active in 11 BioAssays | Tested in 235 BioAssays
CID: 2765
Similar Compounds | Mixture/Component Compounds | BioAssays, activity ≤ 1 µM | PubMed (MeSH Keyword)

24. 

Cocaine muriate; Cocaine chloride; Sal de merck ...
MW: 339.813880 g/mol MF: $C_{17}H_{22}ClNO_4$
IUPAC name: methyl (1R,3R,4S,5S)-3-benzoyloxy-8-methyl-8-azabicyclo[3.2....
CID: 644270
Similar Compounds | Same Parent, Connectivity | Mixture/Component Compounds | PubMed (MeSH Keyword)

25. 

ARGIPRESSIN; Arginine vasopressin; [Arg8]-Vasopressin ...
MW: 1084.231600 g/mol MF: $C_{46}H_{65}N_{15}O_{12}S_2$
IUPAC name: (2S)-1-[(4R,7S,10S,13S,16S,19R)-19-amino-7-(2-amino-2-oxoeth...
Active in 2 BioAssays | Tested in 44 BioAssays
CID: 644077
Similar Compounds | Same Parent, Connectivity | Mixture/Component Compounds | BioAssays, activity ≤ 1 µM | PubMed (MeSH Keyword)

26. 

Lysipressin; Lysopressin; Syntopressin ...
MW: 1056.218200 g/mol MF: $C_{46}H_{65}N_{13}O_{12}S_2$
IUPAC name: (2S)-N-[(2S)-6-amino-1-[(2-amino-2-oxoethyl)amino]-1-oxohexa...
CID: 644076
Similar Compounds | Same Parent, Connectivity | Mixture/Component Compounds | PubMed (MeSH Keyword)

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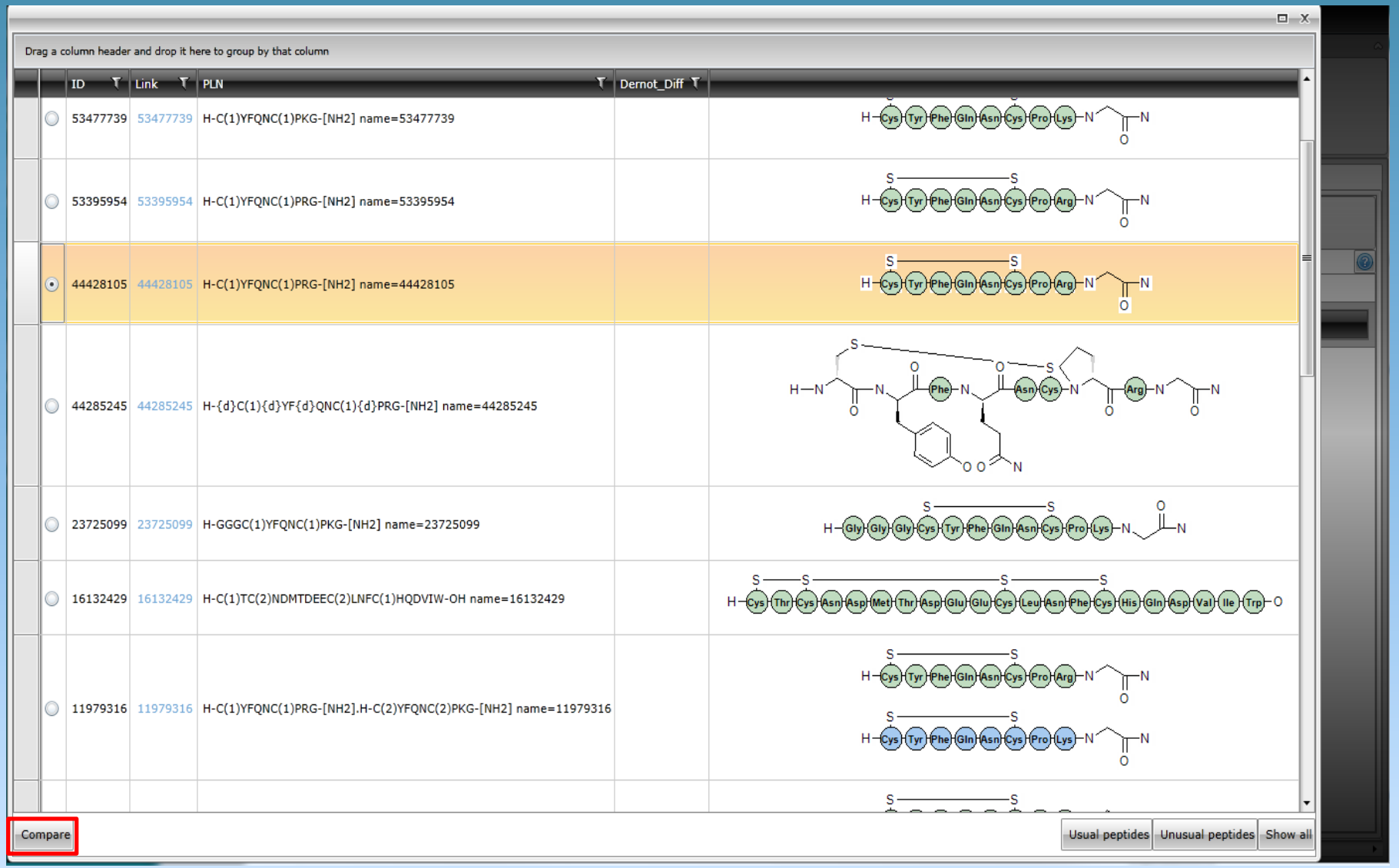
The filtered list only containing peptides in CWM Global Search



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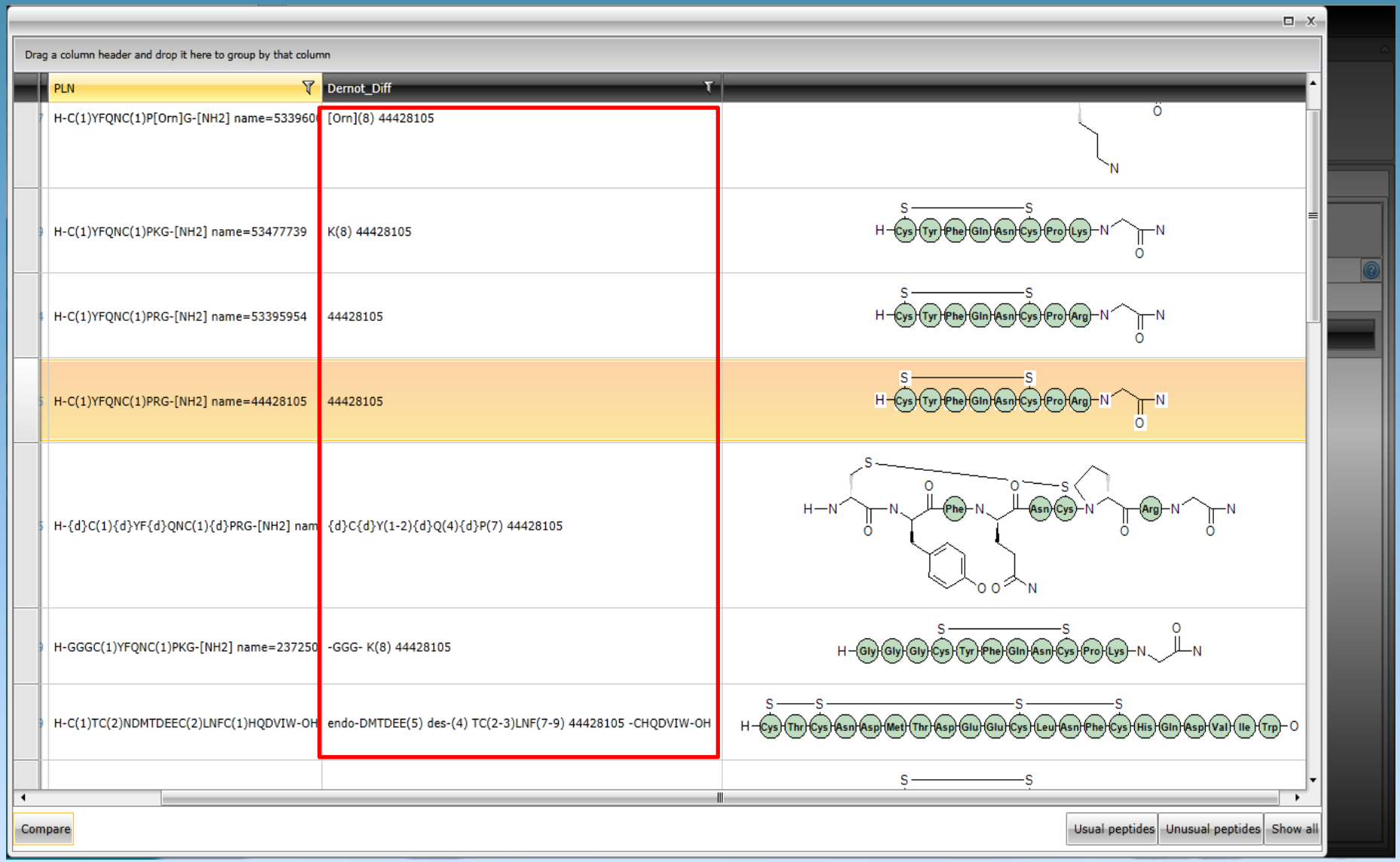
CWM Global Search

The filtered list compared to AVP



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CWM Global Search

Summary :

- CWM Global Search provides an user interface that is as easy to use as Google, but only searches science relevant data sources on the Internet.
- CWM Global Search extend your original query, thus automatically broaden your search.
- Resulting links can, other than Google, be sorted/filtered and grouped, thus making the interpretation of the search results easier for less experienced users.
- Try the FREE version of CWM Global Search at http://cwmglobalsearch.com/gsweb

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CWM Global Search

Summary :

- CWM Global Search professional with Proteax option allows to perform ‚BLAST like' searches in structure centric databases such as ChEBI or PubChem.
- You can use ‚ANY' residues or specific structure fragments to search for unusual peptides.
- ChEBI/PubChem hit lists are ‚mapped back' to three (one) letter sequence codes, thus making the interpretation of results much easier compared with the original database.
- You can filter an arbitrary list of structures to only show peptides and proteins.
- You can easily compare peptides and proteins.

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CWM Global Search

Where can I find more information about CWM Global Search and Proteax ?

- Visit the CWM Global Search home page at http://www.akosgmbh.de/globalsearch
- Visit the Proteax home page at http://www.biochemfusion.com
- Contact us via email globalsearch@akosgmbh.de