

Patents & IP Sequences | Clinical Trials | Drug Pipelines

Creating an Index of Hit Structures using BizInt Smart Charts for Patents

John Willmore, VP Product Development

EPO PIC Workshop, Brussels, 14 November 2018

www.bizint.com

Agenda

- Introduction to BizInt Smart Charts
- Hit structure reports
- Saving and importing transcripts
- Step by step
- Integrating data from separate records

Future directions



We automatically build tabular reports



Integrating results from different databases.

	Drug	Common Drug Name	Database	Synonyms	Highest Phase	Companies	Last Update
1		Pretium					
2	Pretium XGS	Pretium	Loreet Sem	Varius auctor Diam gravida XS-2	Phase2	Lobortis Turpis Aliquam Sodales	2012-10-01
3	Sollicitudin 4S	Sollicitudin	Donec	Quam diam Augue dui	Phase 3	Egestas Condimetum Lobortis Turpis	2011-12-07
4	Sollicitudin	Sollicitudin	Elifend-UR	Quam diam Augue dui Aenean id lectus	Phase 3	Egestas Condimetum	2011-06-07
5	Etiam Mollis	Etiam Mollis	Loreet Sern	Adiscing Proin Mattis Faucibus lasculus	Phase 3	Condimetum Erat	2012-01-13
6	Etiam Mollis	Etiam Mollis	Elifend-UR	Adiscing Et Sec Proin Mattis Faucibus	Phase 2	Condimetum Erat	2012-01-13
7	Toror Felis	Toror Felis	Donec	Aenead lectus purus Nulla sit amet Quisque placerat 2A	Phase 2	Loareet	2011-06-03
8	Toror Felis III	Toror Felis	Loreet Sem	Aenead lectus purus Quisque placerat	Phase 2	Loareet	2011-06-03
9	Consectetur	Consectetur	Donec	Purus non uma Ligula est Quam sem ac	Phase 3	Lobortis turpis	2012-03-01
10	Consectetur 2A	Consectetur	Nullam	Purus non uma Ligula est	Phase 3	Lobortis turpis	2012-03-01

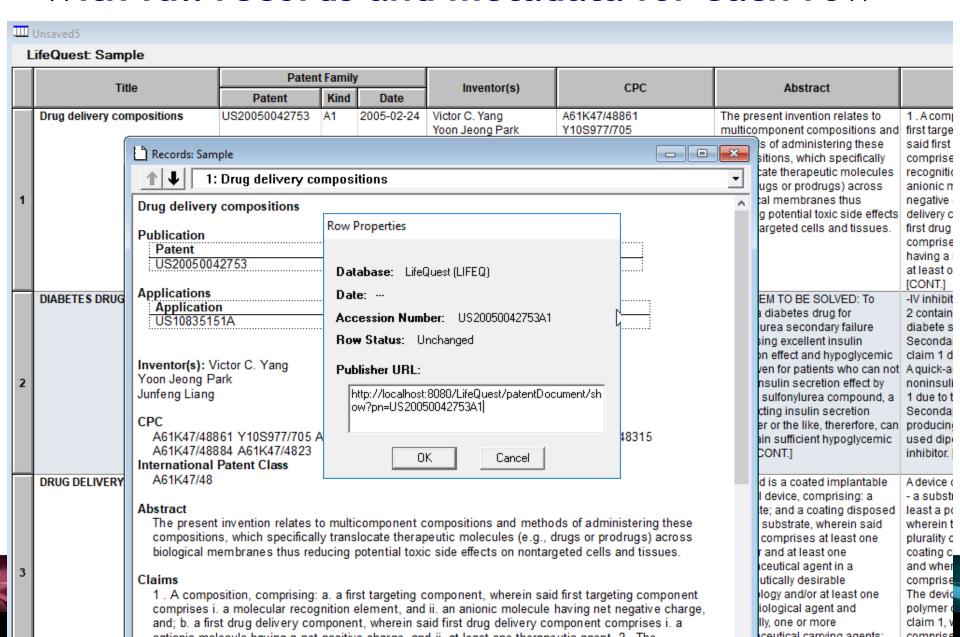
Quickly create tabular reports...



1 25-4	A			
LITE	Ques	E 5	amp	ıe

	Title	Patent Family			Inventor(s) CPC		Abstract	Claims	Pub.
	nue	Patent	Kind	Date	inventor(s)	CPC	Abstract	Ciainis	Fub.
1	Drug delivery compositions	US20050042753	A1	2005-02-24	Victor C. Yang Yoon Jeong Park Junfeng Liang	A61K47/48861 Y10S977/705 A61K2039/505 A61K47/48561 A61K47/48407 A61K47/48315 A61K47/48884 A61K47/4823	The present invention relates to multicomponent compositions and methods of administering these compositions, which specifically translocate therapeutic molecules (e.g., drugs or prodrugs) across biological membranes thus reducing potential toxic side effects on nontargeted cells and tissues.	first drug delivery component comprises i. a cationic molecule having a net positive charge, and ii. at least one therapeutic agent. [CONT.]	
2	DIABETES DRUG	JP2005126430	Α	2005-05-19	ASAKAWA TOMOKO		PROBLEM TO BE SOLVED: To obtain a diabetes drug for sulfonylurea secondary failure expressing excellent insulin secretion effect and hypoglycemic effect even for patients who can not obtain insulin secretion effect by using a sulfonylurea compound, a quick-acting insulin secretion promoter or the like, therefore, can not obtain sufficient hypoglycemic effect. [CONT.]	noninsulin secretagougue of claim 1 due to the described. Secondary diabete [] 2 for	
3	DRUG DELIVERY MEDICAL DEVICE	CA2756386	A1	2010-09-30	NEET, JOHN TAYLOR, DOUGLAS MCCLAIN, JAMES B.	A61M25/0045 A61L2420/08 A61L29/085 A61L2300/63 A61L29/16 A61L2300/602 A61L31/16 A61L31/10 A61L2300/608 A61L27/34 A61L27/16	Provided is a coated implantable medical device, comprising: a substrate; and a coating disposed on said substrate, wherein said coating comprises at least one polymer and at least one pharmaceutical agent in a therapeutically desirable morphology and/or at least one active biological agent and optionally. one or more	A device comprising: - a substrate and - a coating on at least a portion of the substrate, wherein the coating comprises a plurality of layers, wherein the coating comprises an active agent, and wherein the polymer comprises a durable polymer. The device of claim 1, wherein the polymer comprises The device of claim 1. wherein the polymer	Application

With full records and metadata for each row



How is this different from Excel?

- Customize after creation
- Tables within cells
- Images in cells
- Rows sort properly
- Integrate data from different platforms into a single report
- Update reports with new and changed data
- Deliver final reports in HTML, Word, Excel, PDF



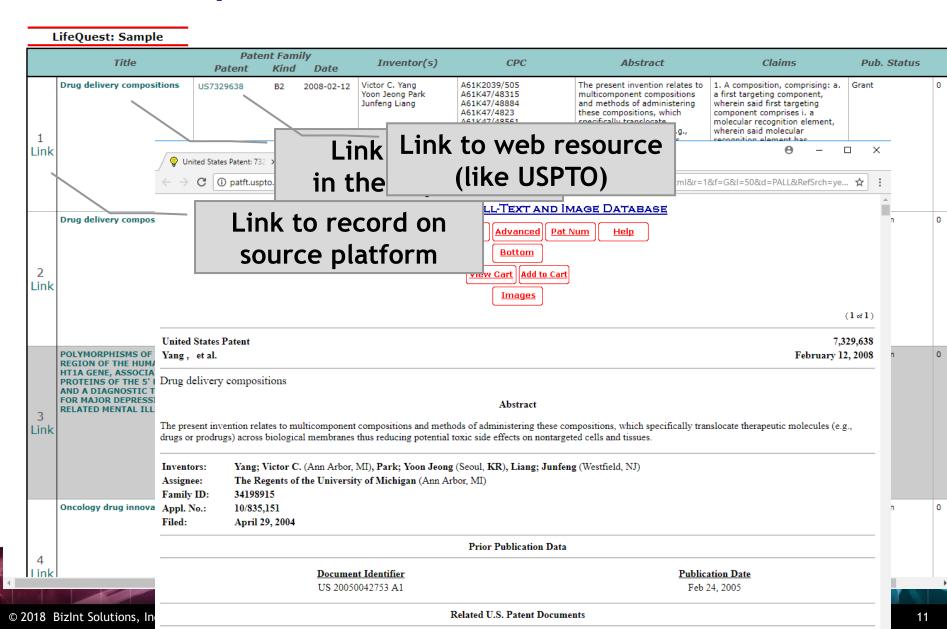
Customize your reports

- Select and rearrange columns
- Add your own columns.
- Create and apply chart templates.
- Hide rows that aren't of interest.
- Sort by multiple values, move rows.
- Edit text and highlight cells.
- Change options for truncation and full text links.
- Tools | Statistics: simple statistics can help analyze search results.

Deliver attractive and useful reports

- Export to HTML, Word, and Acrobat chart only or chart and linked records.
- Export to Excel optimized Excel export, also HTML and .csv exports.
- BizInt Smart Charts files (.chp) consider the Viewer for "aggressive end users".
- Printing (options under Page Setup)

Deliver reports in HTML, Word, Excel...



Summary Record export in Word

3. Basic Patent Number: WO2012033858A2

Title: Boron-containing small molecules

Inventor(s): Hernandez, Vincent S.; Ding, Charles; Plattner, Jacob J.; Alley, Michael Richard Kevin;

Rock, Fernando; Zhang, Suoming; Easom, Eric; Li, Xianfeng; Zhou, Ding

Patent Assignee: Anacor Pharmaceuticals, Inc., USA

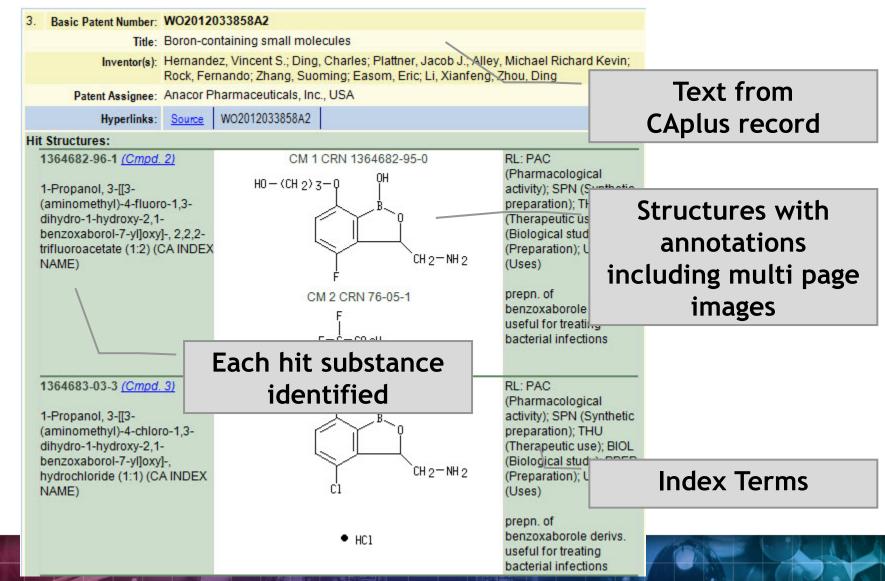
Hyperlinks: Source WO2012033858A2



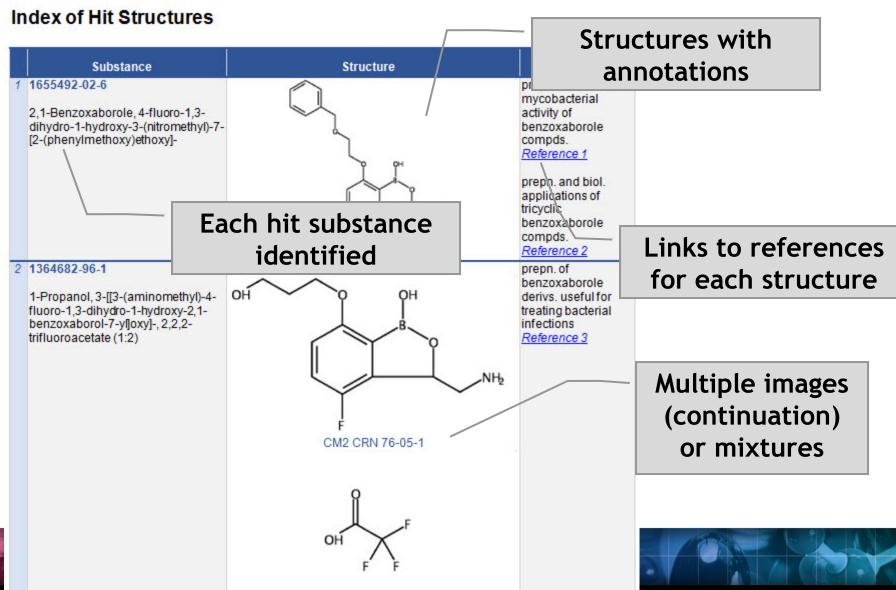
- Fields are the columns in chart
- Content, like hyperlinks, is included in the Summary Record

THE JOURNEY BEGINS...

Summary Record export with Hit Structures

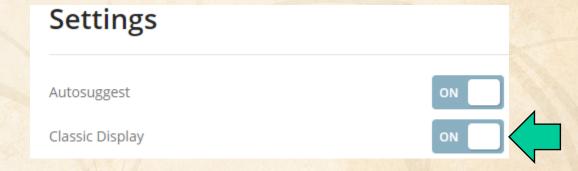


A structure oriented "Index of Hit Structures"



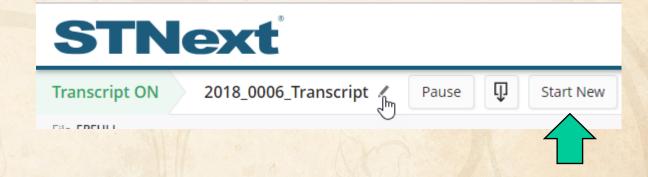
Importing transcripts with hit structures (STNext)

Make sure that Classic Display is on



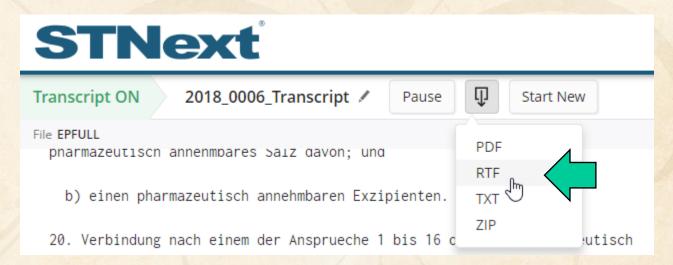
Importing transcripts with hit structures (STNext)

- Make sure that Classic Display is on
- Start new transcript before displaying.



Importing transcripts with hit structures (STNext)

- Make sure that Classic Display is on
- Start new transcript before displaying.
- Display your results including HITSTR.
- Save as RTF.



BIB vs. IBIB

- We recommend using tagged (BIB), rather than indented (IBIB), display formats
- Some field contents (table headings) appear before the label in IBIB
- Indent levels in RTF are more reliably detected in BIB

Importing transcripts with hit structures (other platforms)

New STN: BizInt export - must include both REGISTRY and CAplus records in export

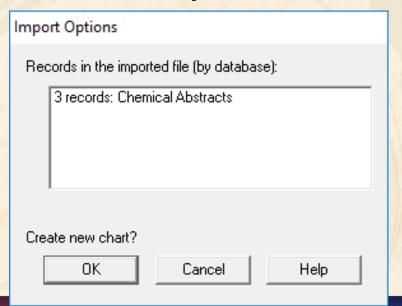
http://www.bizint.com/support/create/newstn_hitstr.php

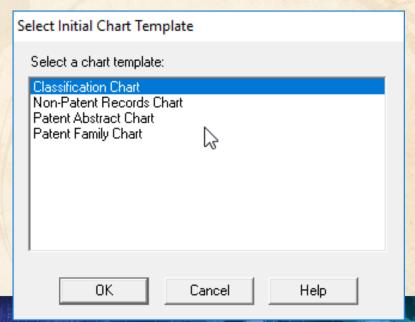
Classic STN: Using STN Express, display HITSTR, save transcript as RTF.

If transcript opens in Word DO NOT SAVE!

Import your transcript

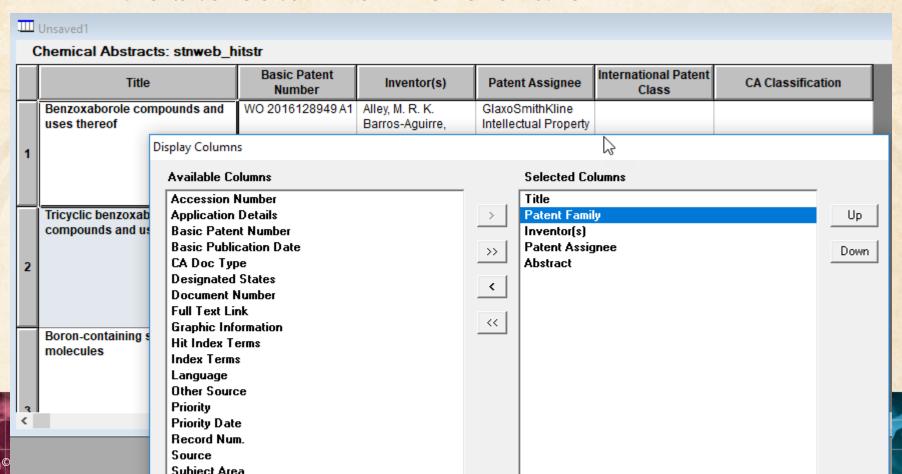
- Either File | Import or drag your transcript file into BizInt Smart Charts for Patents.
- Chart template is a default set of columns Create your own!





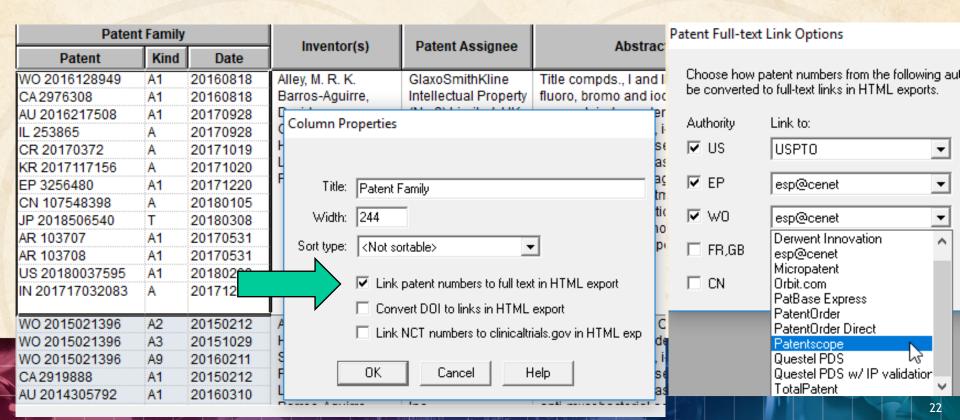
Select columns to display

Use View | Columns to select and re-order visible columns in the chart



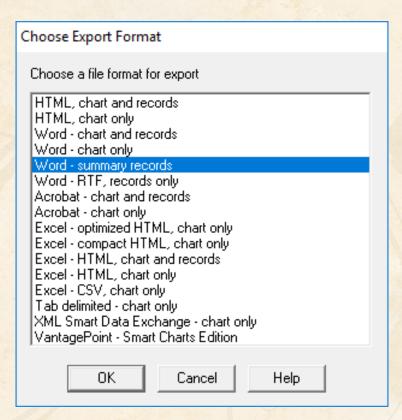
Set column properties

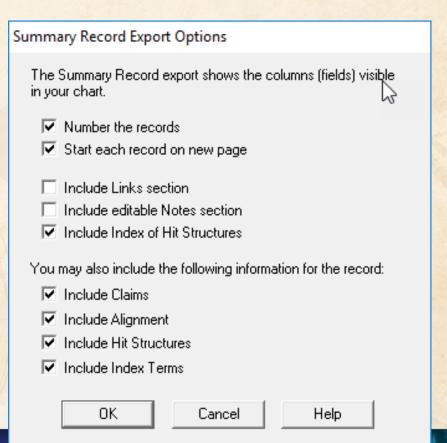
- Use View | Column Properties to change column names or set up hyperlinks
- Configure with Options | Full text patent links



Export to see hit structures

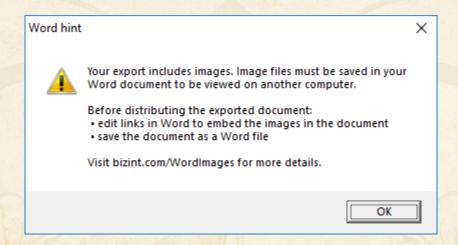
File | Export and choose Word - Summary Records





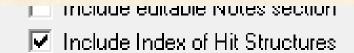
Export to see hit structures

Tip: Structure images are linked in the exported file - you need to embed images and Save As before sending the exported Word document



Option: Index of Hit Structures



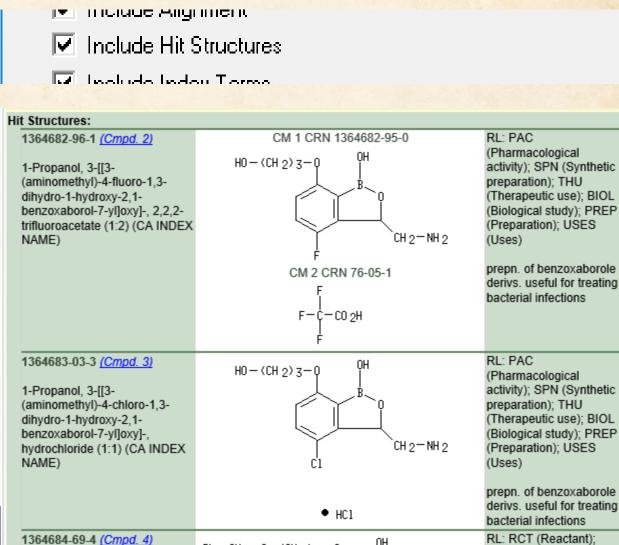


Index of Hit Structures

	Substance	Structure	Reference
1	1655492-02-6 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-(nitromethyl)-7-[2- (phenylmethoxy)ethoxy]- (CA INDEX NAME)	Ph-CH ₂ -0-CH ₂ -CH ₂ -0 OH B O CH ₂ -NO ₂	prepn. and anti- mycobacterial activity of benzoxaborole compds. Reference 1 prepn. and biol. applications of tricyclic benzoxaborole compds. Reference 2
2	1364682-96-1 1-Propanol, 3-[[3-(aminomethyl)-4-fluoro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)	CM 1 CRN 1364682-95-0 H0 - (CH ₂) ₃ -0 CH ₂ -NH ₂ CM 2 CRN 76-05-1 F-C-C0 ₂ H	prepn. of benzoxaborole derivs. useful for treating bacterial infections Reference 3

Option: Hit Structures





 $Ph - CH_2 - 0 - (CH_2)_3 - Q$

2,1-Benzoxaborole, 4-fluoro-1,3-

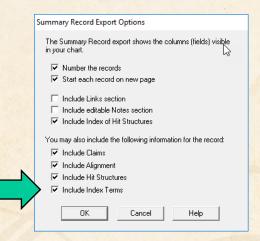
dihvdro-1-hvdroxy-3-

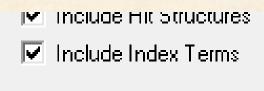
SPN (Synthetic preparation); PREP

(Preparation): RACT



Option: Index Terms





Index Terms:

1364682-96-1P (Cmpd. 2) 1364683-03-3P (Cmpd. 3) PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of benzoxaborole derivs. useful for treating bacterial infections)

1364684-69-4P (Cmpd. 4) 1364684-75-2P (Cmpd. 5) RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of benzoxaborole derivs. useful for treating bacterial infections)

Integrating data from separate records

Reference Rows is a utility to combine multiple records from the same family into one "row" Records grouped by "Common Family" Matching publication numbers in the family

Create reports integrating key IP data...

CAS-9 - GenomeQuest, PatBase, DWPI (new STN), FAMPAT

Title	Title Database _			Patent Family			Family Status				Sequence I	ocations	,	
Title	Database	Patent	Kind	Date	Pub No.	State	Status	Expiry	Probable Assignee	Seq. ID Number	% Identity	Length	Location	
1. Modulating expression of a target nucleic acid comprises providing to the cell a guide RNA including a transcriptional activator or repressor domain as a fusion protein, and providing to the cell a nuclease null Cas9 protein	1.1 DWPI 1.2 DWPI 1.3 GPATPRT link 1.4 GPATPRT link 1.5 Patbase link 1.6 FAMPAT link	US 2014356959 US 2014356956 AU 2014274939 WO 14197568 WO 14197568 CA 2914638 KR 20160014036	A AA A2 A3 AA	2014-12-11 2014-12-11 2015-03-12	US 20140356956 A1 US 9267135 B2			2034-06-04	PRESIDENT AND FELLOWS OF HARVARD COLLEGE	US20140356959-0001	100.00	1368 1368	probable disclosure (not found by automated parsing) probable disclosure (not found by automated parsing)	
1.1 DWPI				1.5 Patbase				1.6 FAMPAT	1.5 Patbase					
2. New bacteriophage comprises polynucleotide expressing RNA-directed DNA-binding polypeptide comprising nuclease module, and targeting module comprising guide RNA, for restricting growth of host cell, and for preparing antiseptic composition	2.1 DWPI 2.2 DWPI 2.3 GPATPRT link 2.4 GPATPRT link 2.5 Patbase link 2.6 FAMPAT link	WO 15070193 US 2015132263 US 2015353901	Α	2015-05-14 2015-05-14 2015-12-10	WO 201570193 A1 US 20150132263 A1 US 20150353901 A1	ALIVE ALIVE	PENDING	2034-11-11 2034-11-11 2034-11-11	RADIANT GENOMICS INC	US20150132263-0002 US20150353901-0002	100.00	1368 1368	claim: 19; 20 claim: 19; 20	2.3

2.1 DWPI

choosing content by rules...

	Title	Database	Patent Family					
	nue	Database	Patent	Kind	Date			
1.	Modulating expression of a target nucleic acid comprises providing to the cell a guide RNA including a transcriptional activator or repressor domain as a fusion protein, and providing to the cell a nuclease null Cas9 protein	1.1 DWPI 1.2 DWPI 1.3 GPATPRT link 1.4 GPATPRT link 1.5 Patbase link 1.6 FAMPAT link	US 2014356959 US 2014356956 AU 2014274939 WO 14197568 WO 14197568 CA 2914638 KR 20160014036	A A AA A2 A3 AA A	2014-12-04 2014-12-04 2014-12-11 2014-12-11 2015-03-12 2015-12-04 2016-02-05			
	1.1 DWPI				1.5 Patbas			
2.	New bacter iophage comprising RNA-directed DNA-binding polypeptide comprising nuclease module, and targeting module comprising guide RNA, for restricting growth of host cell, and for preparing antiseptic composition	2.1 DWPI 2.2 DWPI 2.3 GPATPRT link 2.4 GPATPRT link 2.5 Patbase link 2.6 FAMPAT link	WO 15070193 US 2015132263 US 2015353901	A1	2015-05-14 2015-05-14 2015-12-10			
	2.1 DWPI				2.5 Patbas			

linking unique content...

	Fami	ily Status		Probable Assignee
Pub No.	State	Status	Expiry	1 Tobable Assignee
US 20140356956 A1 US 9267135 B2			2034-06-04	PRESIDENT AND FELLOWS OF HARVARD COLLEGE
WO 201570193 A1 US	AL AL		1.6 FAMPAT 2034-11-11 2034-11-11	RADIAN NOMICS INC
20150132263 A1 US 20150353901 A1	ALIVE		2034-11-11	
			2.6 FAMPAT	2.5 Patbase

...and summarizing data elements.

		4.5		- 13
S	equence L	ocations.	;	
Seq. ID Number	% Identity	Length	Location	
US20140356959-0001	100.00	1368	probable disclosure (not found by automated parsing)	1.3
US20140356956-0001	100.00	1368	probable disclosure (not found by automated parsing)	1.4
US20150132263-0002	100.00	-8	claim: 19; 20	2.3
US20150353901-0002	100.00	68	claim: 19; 20	2.4



BizInt Smart Charts



for Patents

Patent Databases

Provide data on patents filed worldwide

- STN Classic, STNext, & New STN
- Questel Orbit.com
- Minesoft PatBase
- Innovation, Cortellis IP, Integrity Patents
- LexisNexis TotalPatent
- GQ LifeSciences LifeQuest



BizInt Smart Charts



for Patents

STN Content

- DWPI, IFI, Caplus, MARPAT, REGISTRY
- Fulltext: US PCT EP JP KR AU CA CN FR GB DE
- Literature: EMBASE, MEDLINE, BIOSIS, AGRICOLA, ANABSTR, AQUASCI, BIOENG, BIOTECHNO, CABA, CANCERLIT, COMPENDEX, COMPUAB, COMPUSCIENCE, DISSABS, ENCOMPLIT, FEDRIP, FSTA, FROSTI, INSPEC, IPA, KOSMET, LIFESCI, METADEX, PASCAL, RAPRA, SciSearch, TOXCENTER, TULSA, GEOREF, PQSciTech, DDF
- Sequence: DGENE, PCTGENE, USGENE

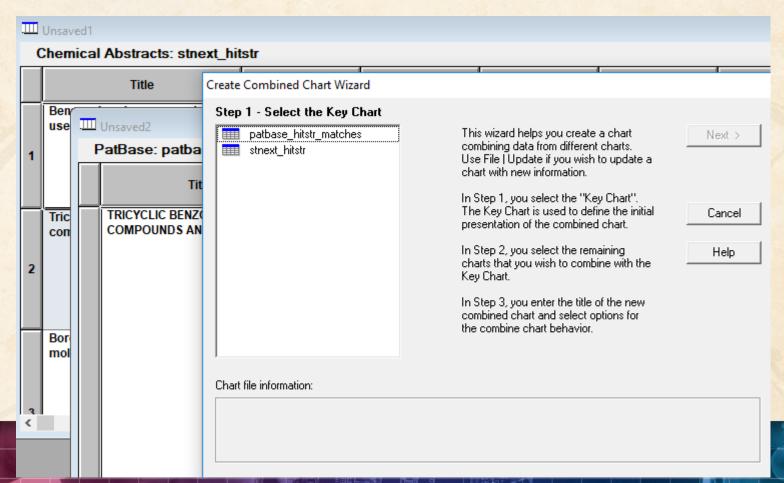
Hit structures in Reference Rows

Reference Rows is a utility to combine multiple records from the same family into one "row" Records grouped by "Common Family" Matching publication numbers in the family Uses:

Add claims from other sources

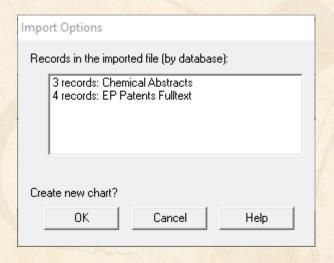
Add claims from other sources

Combine results from two or more databases



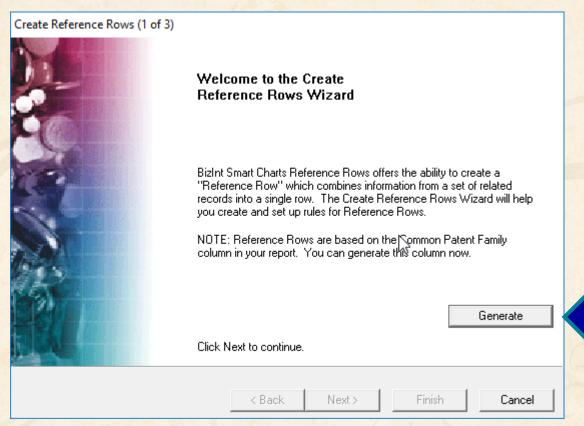
Add claims from other sources

Or import a multi-file transcript file epfull transfer pn 12 1-...

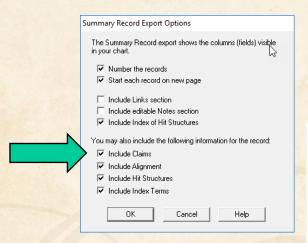


Add claims from other sources

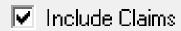
Send to Reference Rows



Option: Claims + Hit Structures



You may also include the following information for the record:



Tall the all the Alberta and the

10. An in vitro method of:

- (A) inhibiting an enzyme, comprising: contacting the enzyme with the compound of any of claims 1 to.5, thereby inhibiting the enzyme:
- (B) killing and/or preventing the growth of a microorganism, comprising; contacting the microorganism with an effective amount of the compound of any of claims 1 to 5, thereby killing and/or preventing the growth of the microorganism; or
- (C) inhibiting the editing domain of a t-RNA synthetase, comprising; contacting the synthetase with an effective amount of a compound of any of claims 1 to 5, or a pharmaceutically-acceptable salt thereof, thereby inhibiting the synthetase.

Hit Structures:

1364682-96-1 (Cmpd. 2)

1-Propanol, 3-[[3-(aminomethyl)-4-fluoro-1,3dihydro-1-hydroxy-2,1benzoxaborol-7-yl]oxy]-, 2,2,2trifluoroacetate (1:2) (CA INDEX NAME)

CM 1 CRN 1364682-95-0

CM 2 CRN 76-05-1

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

prepn. of benzoxaborole derivs, useful for treating bacterial infections



© 2018 BizInt Solutions, Inc | www.bizint.com

1364683-03-3 (Cmpd. 3)

RL: PAC

Hit structures in Reference Rows

Reference Rows is a utility to combine multiple records from the same family into one "row" Records grouped by "Common Family" Matching publication numbers in the family Uses:

- Add claims from other sources
- Link sequence results with hit structures



BizInt Smart Charts



for Patents

IP Sequence Databases

Provide data on sequences filed in patents

- GenomeQuest (Geneseq, GQ-PAT)
- STN (USGENE, DGENE, PCTGEN)

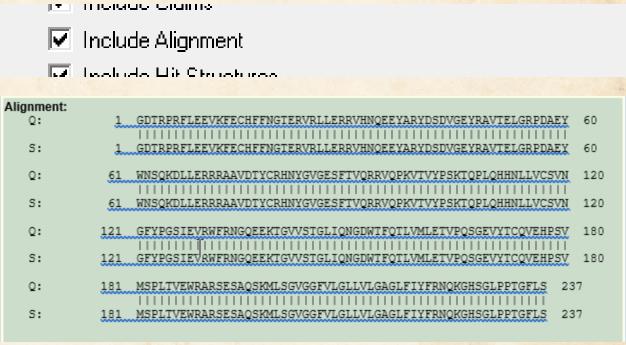
Link sequence results with hit structures

Follow Cookbook recipe to create a summary of sequence hits for each

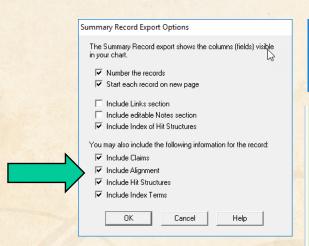
1.	Title:	Selective high-affinity	polydentate	ligands and	methods of making such
	Database:	GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins Chemical Abstracts Chemical Abstracts			
	Organism Species:	Homo sapiens (human)			
	Sequence Summary:	Seq. ID Number	Length	% Identity	Location
		US20180008621-0003	237	100.00	probable disclosure (not found by automated parsing)
		US9884070-0003	237	100.00	probable disclosure (not found by automated parsing)
		US20180008622-0003	237	100.00	probable disclosure (not found by automated parsing)
		JP5623384-0003	237	100.00	probable disclosure (not found by automated parsing)
		JP2014122234-0003	237	100.00	probable disclosure (not found by automated parsing)
		US20110144065-0003	237	100.00	probable disclosure (not found by automated parsing)
		CA2721980-0003	237	100.00	probable disclosure (not found by

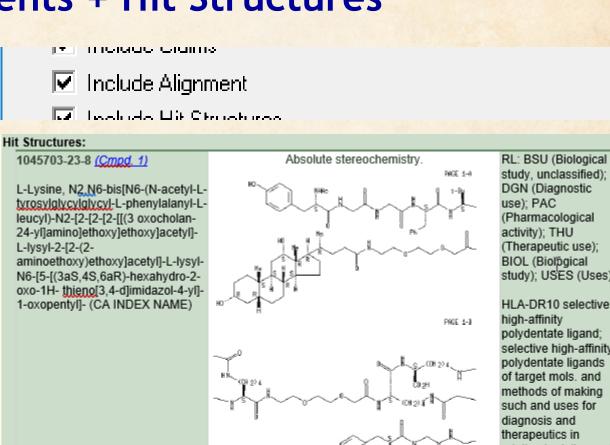
Option: Alignments + Hit Structures





Option: Alignments + Hit Structures

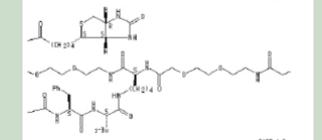




study, unclassified); DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use): BIOL (Biological study); USES (Uses)

HLA-DR10 selective high-affinity polydentate ligand; selective high-affinity polydentate ligands of target mols. and methods of making such and uses for diagnosis and therapeutics in relation to delivery of effectors

PAGE 1-C



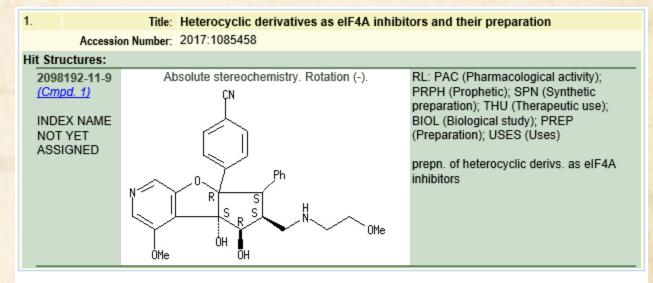
Hit structures in Reference Rows

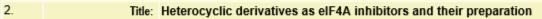
Reference Rows is a utility to combine multiple records from the same family into one "row" Records grouped by "Common Family" Matching publication numbers in the family Uses:

- Add claims from other sources
- Link sequence results with hit structures
- Merge hit structures spread across multiple CAplus records ("mega-TAN" records)

Group Mega-TAN records

Multiple CA records for a single family...





Accession Number: 2017:1085457

Hit Structures:

2099275-30-4 (Cmpd. 2)

INDEX NAME NOT YET ASSIGNED

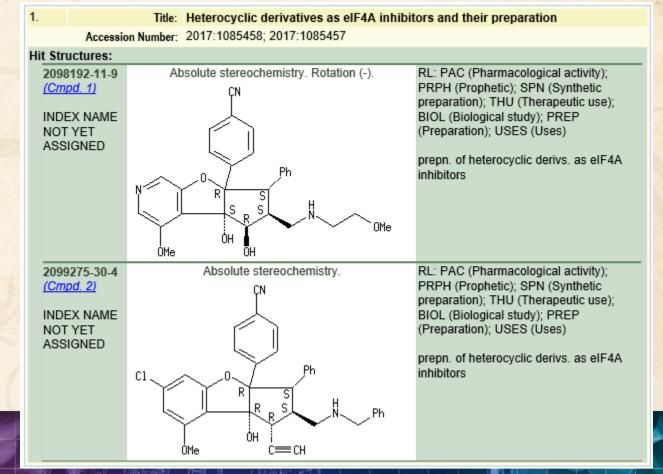
Absolute stereochemistry.

RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

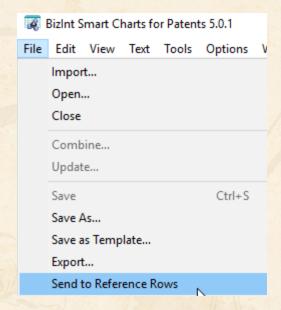
prepn. of heterocyclic derivs. as eIF4A inhibitors

Group Mega-TAN records

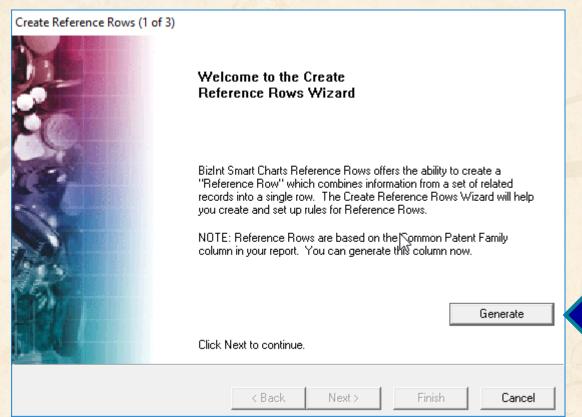
Simply send to Reference Rows and export!



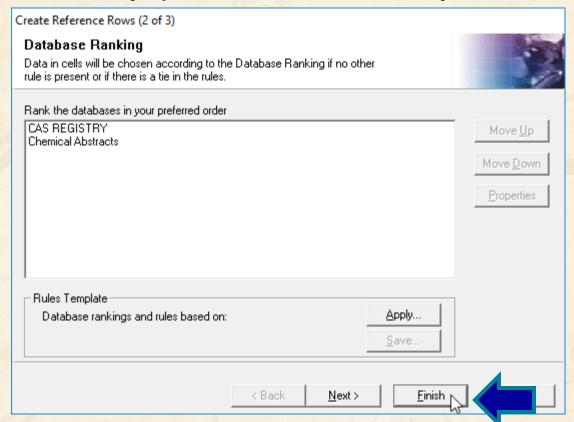
- Save chart in BizInt Smart Charts for Patents
- Send to Reference Rows



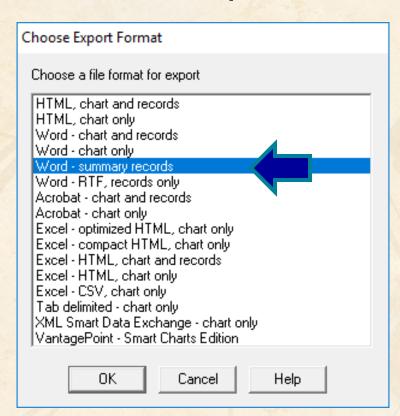
Generate Common Patent Family (if needed)



Simply "Finish" on step two

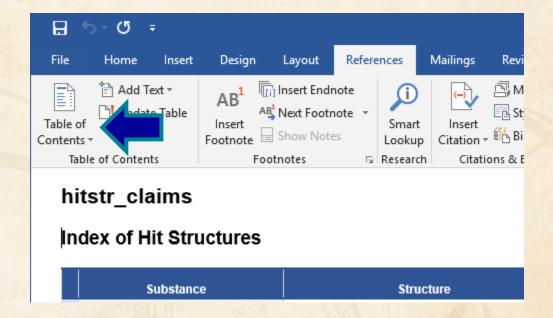


File | Export ... Word - summary records



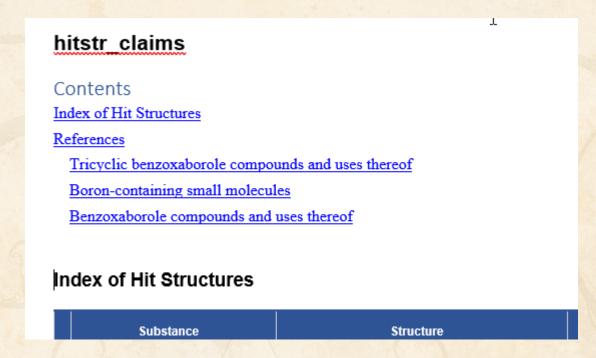
Summary Records - Table of Contents

Add a table of contents in Word



Summary Records - Table of Contents

- Sections are marked up for headings
- First column in chart is used as TOC entry



Summary Records - Table of Contents

 Can collapse the Index of Hit Structures (in recent versions of Word)

```
References

1. Title: Tricyclic benzoxaborole compounds and uses thereof
Common Family: EP 3030519

Database: Chemical Abstracts
EP Patents Fulltext

Patent Family: Patent Kind Date
WO 2015021396 A2 20150212
WO 2015021396 A3 20151029
```

- Typical use as described by Marley at PIUG 2018 Annual Meeting is to display structures exemplified in CAplus records (the Index of Hit Structures)
- Plus a separate table of non-exemplified structures from REGISTRY
- Today, this should be done as two chart files
- Also, today we do not capture complex structures from REGISTRY

- The hit structure displays are driven by the "Hit Index Terms" column
- You can remove a compound from the hit structure display and the index by removing the CAS REGISTRY Number from the Hit Index

Terms column

	Hit Index Terms					
	RN	Role	Notes			
		RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)	prepn. of benzoxaborole derivs. useful for treating bacterial infections			
		RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)	prepn. of benzoxaborole derivs. useful for treating bacterial infections			

- Keep your transcripts!
- As we improve displays, some features may require re-importing transcripts.

- Keep your chart files!
- Even though you may have delivered a report to your client, if they ask for changes (additional fields, different sort order) it is easier to start from a prepared chart than from scratch.

- Keep your chart files!
- This month's report can be the baseline for an updated report.
- You can Update a report to see which families are new in your results and which

have changed.

PatBase: Natamycin_Update									
	T:41-	Row Status	Patent Family		Priority Data		Applications		
	Title		Patent	Kind	Date	Number	Date	Application	Date
2	SUBMICRON NATAMYCIN PARTICLE	Added	WO 15044465 WO 15044465	A2 A3		EP20140167408 EP20140192514	2014-05-07 2014-11-10	W02015EP50647 W02015EP50647	2015-01-15 2015-01-15
3	COMPOSITION COMPRISING A PESTICIDAL TERPENE MIXTURE AND A FUNGICIDE	Updated	WO 14020109 AU 2013298562 CA 2880671 AR 091953 KR 20150041638	A1 AA AA AA	2014-02-06 2014-02-06 2015-01-30 2015-03-11 2015-04-16	EP20120179145 WO2013EP66178	2012-08-03 2013-08-01	W02013EP66178 AU20130298562 CA20132880671 AR2013P102729 KR20157004997	2013-08-01 2013-08-01 2013-08-01 2013-08-01 2013-08-01

Future Directions

- Options to control display
- Mark new structures in updated reports
- More sources (e.g. MARPAT, DWPIM)
- Handling of complex structures in REGISTRY
- More export formats
- Hit structures in the table

