

Patents & IP Sequences | Clinical Trials | Drug Pipelines

# **Creating an Index of Hit Structures with BizInt Smart Charts for Patents and STNext**

John Willmore, VP Product Development 8 October 2018

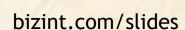
www.bizint.com



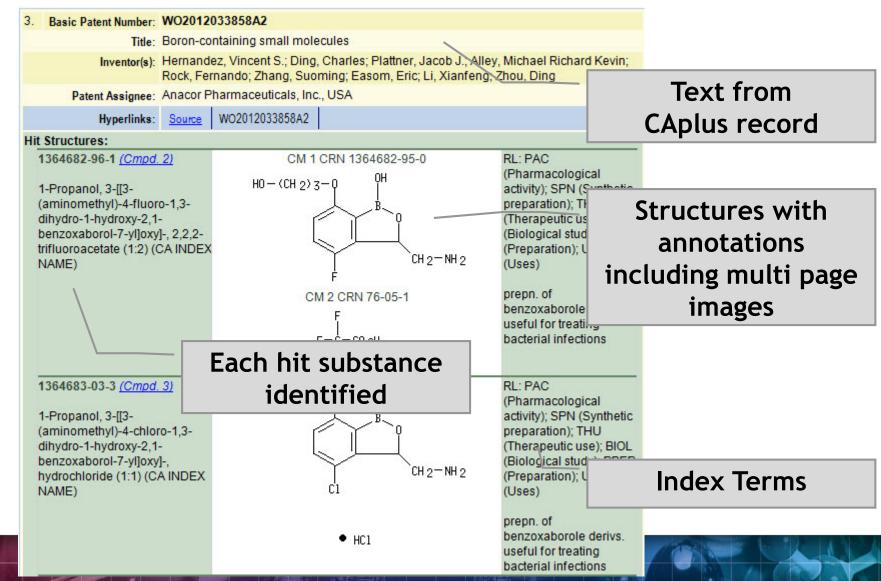
# Agenda

- Hit structure reports
- Saving and importing transcripts
- Step by step
- Integrating data from separate records

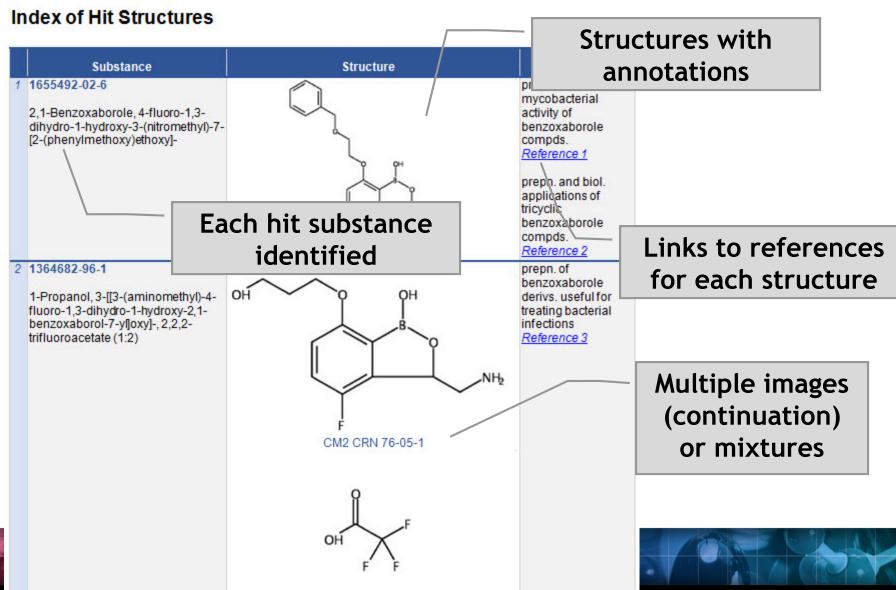
Future directions



# Summary Record export with Hit Structures

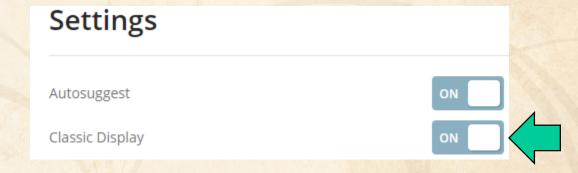


### A structure oriented "Index of Hit Structures"



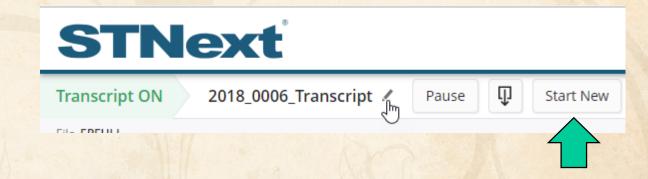
# Importing transcripts with hit structures (STNext)

Make sure that Classic Display is on



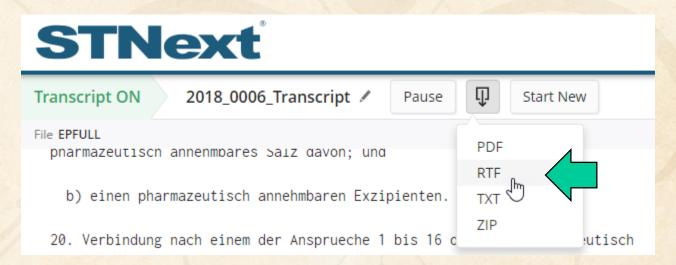
# Importing transcripts with hit structures (STNext)

- 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.



# Importing transcripts with hit structures (other platforms)

http://www.bizint.com/support/create/newstn\_hitstr.php

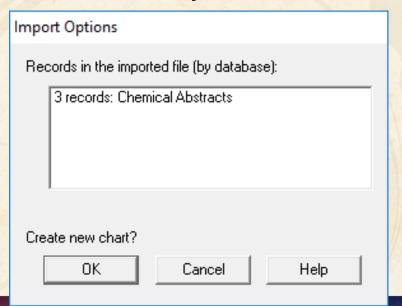
New STN: BizInt export - must include both REGISTRY and CAplus records in export

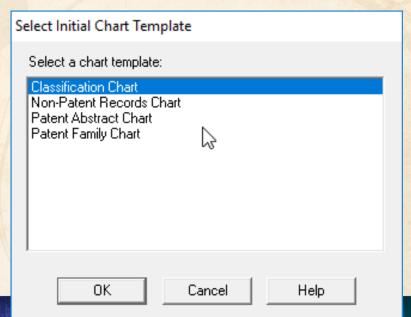
Classic STN: Using STN Express, display HITSTR, save transcript as RTF.

If transcript opens in Word DO NOT SAVE!

# Import your transcript

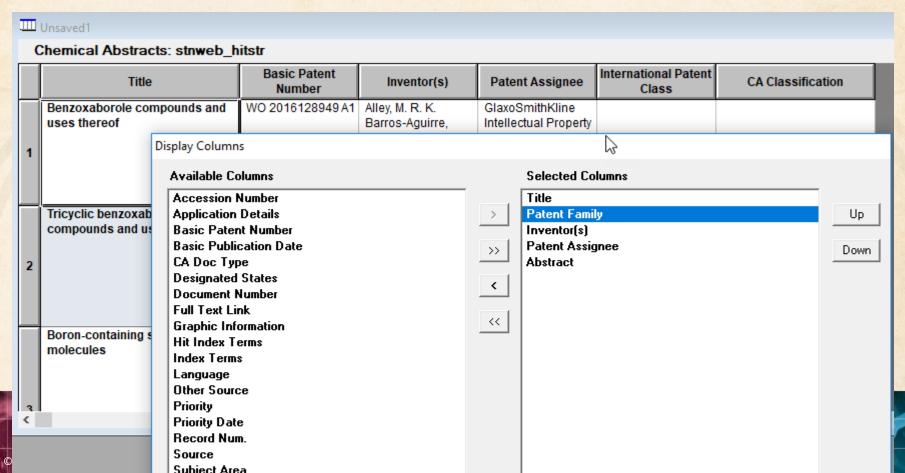
- Either File | Import or drag your transcript file into BizInt Smart Charts for Patents.
- Chart template is a default set of columns Create your own!





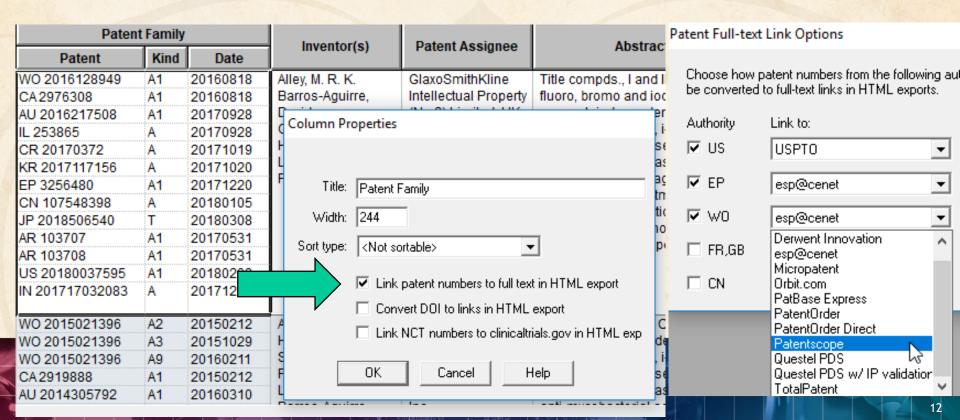
# Select columns to display

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



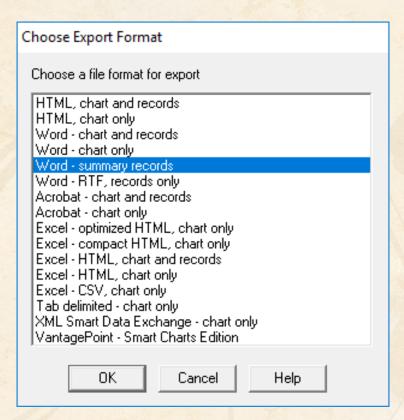
# Set column properties

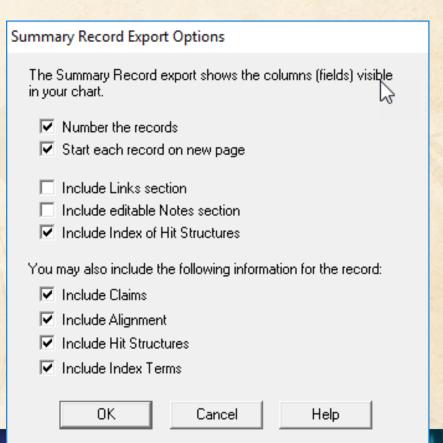
- Use View | Column Properties to change column names or set up hyperlinks
- Configure with Options | Full text patent links



# Export to see hit structures

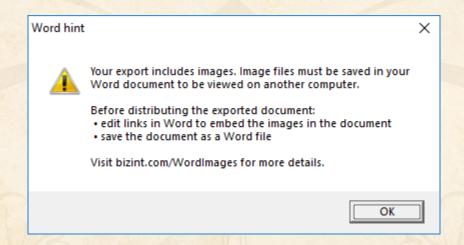
# File | Export and choose Word - Summary Records





# Export to see hit structures

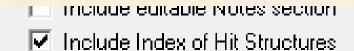
Tip: Structure images are linked in the exported file - you need to embed images and Save As before sending the exported Word document



# **Option: Index of Hit Structures**



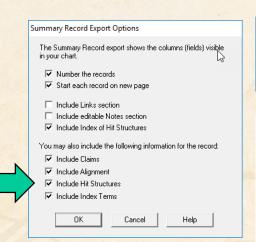
© 2018 BizInt Solutions, Inc | www.bizint.com

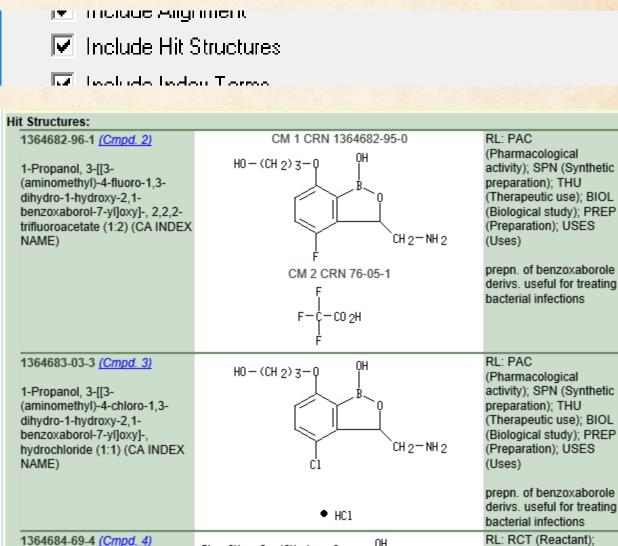


#### Index of Hit Structures

	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 <sub>2</sub> -0-CH <sub>2</sub> -CH <sub>2</sub> -0 OH B O CH <sub>2</sub> -NO <sub>2</sub>	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 2H  F	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-

dihydro-1-hydroxy-3-

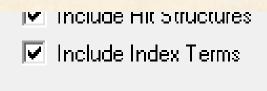
SPN (Synthetic preparation); PREP

(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

												7717		
Title	Database	Patent Family		Family Status				Probable Assignee	Sequence Locations					
Title		Patent	Kind	Date	Pub No.	State	Status	Expiry	r Tobable Assignee	Seq. ID Number	% Identity	Length	Location	
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	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 AA AA	2014-12-11 2015-03-12 2015-12-04	US 20140356956 A1 US 9267135 B2			2034-06-04 2034-06-04	PRESIDENT AND FELLOWS OF HARVARD COLLEGE	US20140356959-0001	100.00	1368	probable disclosure (not found by automated parsing) probable disclosure (not found by automated parsing)	
null Cas9 protein									***************************************					
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	2.4

2.1 DWPI

# choosing content by rules...

	Title	Database	Patent Family				
	Title	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 A A A A A 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 bacteriophage 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 Patba		

# 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	AL	PENDING	1.8 FAMPAT 2034-11-11	1.5 Patbase  RADIAN NOMICS INC		
A1 US 20150132263 A1	ALI	PENDING	2034-11-11			
US 20150353901 A1		PENDING	2034-11-11			
			2.6 FAMPAT	2.5 Patbase		

# ...and summarizing data elements.

S	equence L	ocations.	i e	
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

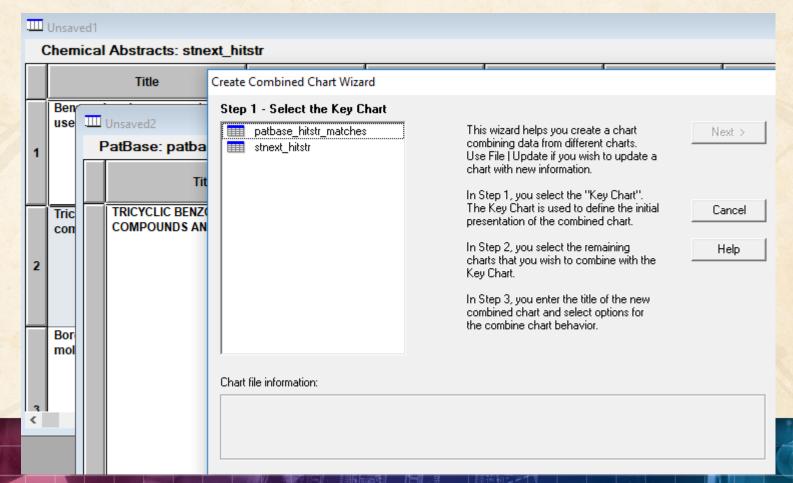
### Hit structures in Reference Rows

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

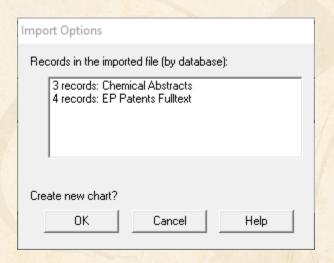
### Add claims from other sources

### Combine results from two or more databases



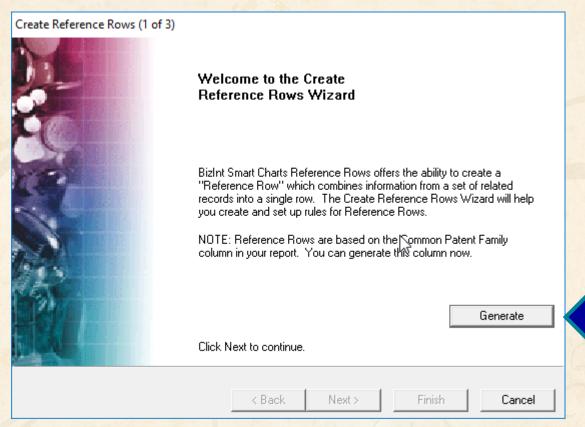
### Add claims from other sources

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

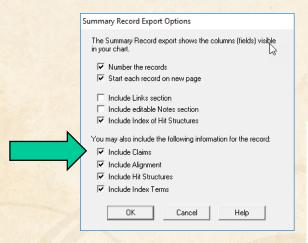


### Add claims from other sources

### Send to Reference Rows



# Option: Claims + Hit Structures



You may also include the following information for the record:



Tall the all that Alliana are to

#### 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

RL: PAC 1364683-03-3 (Cmpd. 3)

### 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

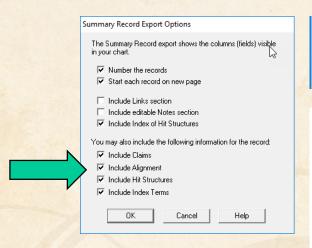
- GenomeQuest (Geneseq, GQ-PAT)
- STN (USGENE, DGENE, PCTGEN)

# Link sequence results with hit structures

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

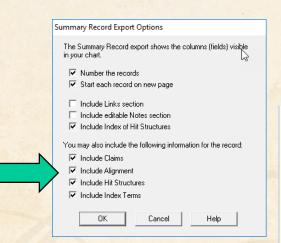
1.	Title:	Selective high-affinity	polydentate	ligands and	methods of making such
	Database:	GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins Chemical Abstracts Chemical Abstracts			
	Organism Species:	Homo 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 automated parsing)

# Option: Alignments + Hit Structures

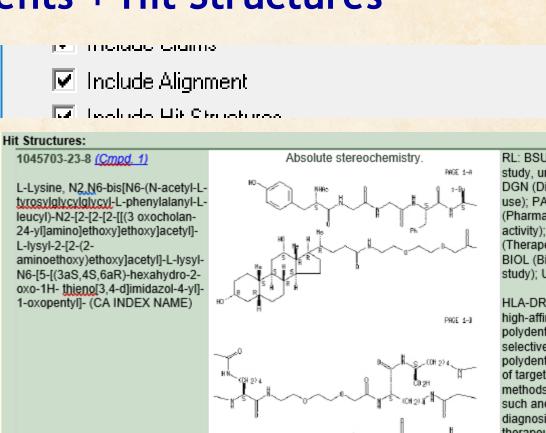


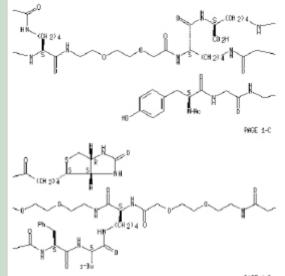


# Option: Alignments + Hit Structures



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





RL: BSU (Biological 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

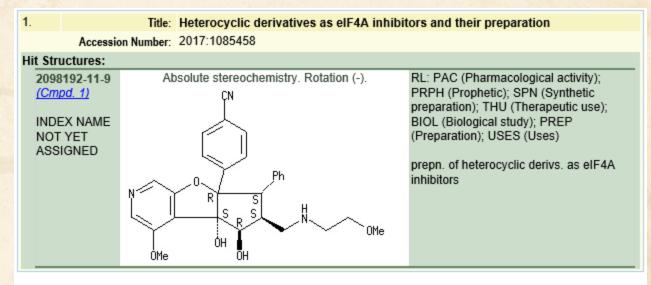
### Hit structures in Reference Rows

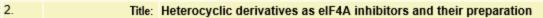
Reference Rows is a utility to combine multiple records from the same family into one "row" Records grouped by "Common Family" Matching publication numbers in the family Uses:

- 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

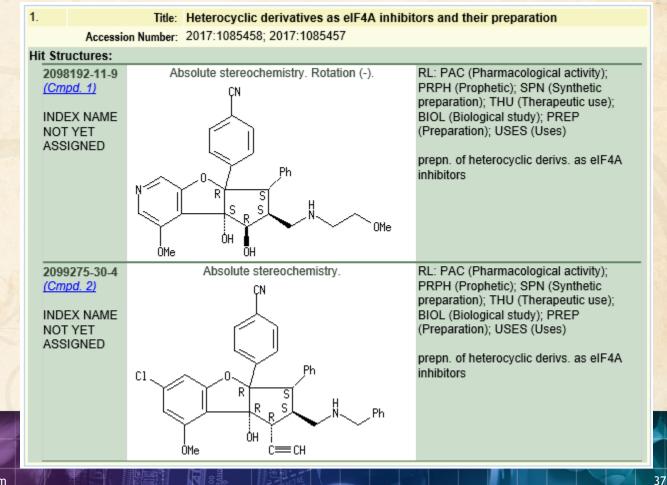
Absolute stereochemistry.

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!



### **Future Directions**

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

