Software for
Business Intelligence

BizInt Smart Charts

Patents & IP Sequences | Clinical Trials | Drug Pipelines

Software for presenting results of chemical structure searches

Matt Eberle

John Willmore, VP Product Development

August 2018

Agenda

- Integrating unique IP information
- Challenges in reporting chemical structure searches
- New solution: summary records with hit structures
- Integrate unique IP information & hit structures
- Future directions
- Questions

BizInt Smart Charts - Integrate unique information from fulltext, family, and IP sequence databases

Title	Family Status				Probable Assignee	Sequence Locations			
	Pub No.	State	Status	Expiry		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 null Cas9 protein									
Altering a target nucleic acid in a cell involves RNAs and Cas9 protein nickase co-localize to DNA target nucleic acid and nick the target nucleic acid resulting in adjacent nicks									
RNA-Guided Transcriptional Regulation	US 20140356956 A1	ALIVE	PENDING	2034-06-04					
	US 9267135 B2	ALIVE	GRANTED	2034-06-04					
RNA-Guided Transcriptional Regulation						US20140356959-0001	100.00	1368	probable disclosure (not found by automated parsing)
RNA-Guided Transcriptional Regulation						US20140356956-0001	100.00	1368	probable disclosure (not found by automated parsing)
RNA-GUIDED TRANSCRIPTIONAL REGULATION					PRESIDENT AND FELLOWS OF HARVARD COLLEGE				

BizInt Smart Charts

Reference Rows™

Reference Rows integrated report

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

	Title	Database	Patent Family			Family Status			
			Patent	Kind	Date	Pub No.	State	Status	Expiry
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	US 2014356959	A	2014-12-04	US 20140356956 A1	ALIVE	PENDING	2034-06-04
		1.2 DWPI	US 2014356956	A	2014-12-04	US 9267135 B2	ALIVE	GRANTED	2034-06-04
		1.3 GPATPRT | *link*	AU 2014274939	AA	2014-12-11				
		1.4 GPATPRT | *link*	WO 14197568	A2	2014-12-11				
		1.5 Patbase | *link*	WO 14197568	A3	2015-03-12				
		1.6 FAMPAT | *link*	CA 2914638	AA	2015-12-04				
	1.1 DWPI		KR 20160014036	A	2016-02-05				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	WO 15070193	A1	2015-05-14	WO 201570193 A1	ALIVE	PENDING	2034-11-11
		2.2 DWPI	US 2015132263	A	2015-05-14	US 20150132263 A1	ALIVE	PENDING	2034-11-11
		2.3 GPATPRT | *link*	US 2015353901	A	2015-12-10	US 20150353901 A1	ALIVE	PENDING	2034-11-11
		2.4 GPATPRT | *link*							
		2.5 Patbase | *link*							
		2.6 FAMPAT | *link*							
	2.1 DWPI								2.6 FAMPAT
			2.5 Patbase						

Challenges in reporting chemical structure searches

- Multiple hit structures per record possible (probable)
- Report options generally record-centric, not structure centric.

That means…

- Transcript and other display options repeat the same structure.
- Structures take up space and not always formatted well – ie page breaks
- Solution is often a lot of manual work

A New Solution for reporting hit structures...

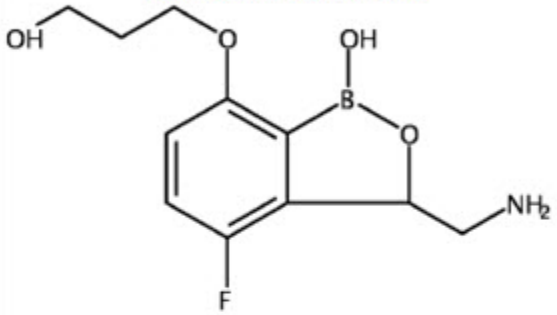
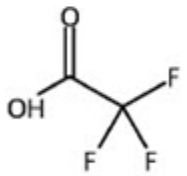
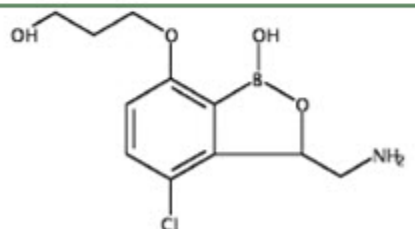
"Exemplified Compounds Table linked to Citing Publications" - presented by Maddy Marley (GSK) at PIUG 2018 Annual Conference, Alexandria, Virginia, May 2018.
bizint.com/slides

Summary Record export with Hit Structures

New STN

3.	**Basic Patent Number:**	**CA2810021A1**
	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., United States (US)
	Hyperlinks:	CA2810021A1

Hit Structures:

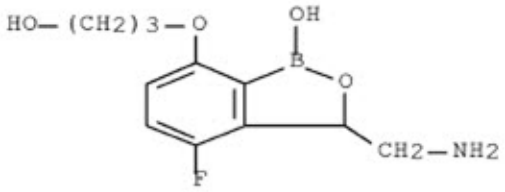
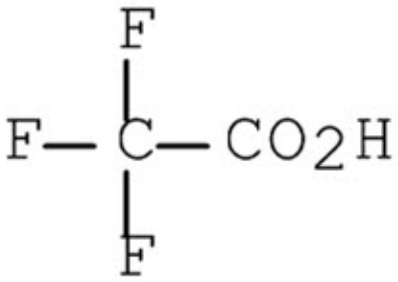
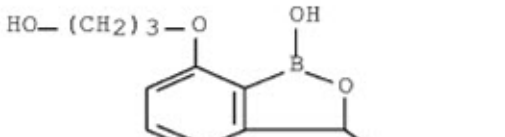
1364682-96-1 *(Cmpd. 2)* 1-Propanol, 3-[[3-(aminomethyl)-4-fluoro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, 2,2,2-trifluoroacetate (1:2)	CM1 CRN 1364682-95-0  CM2 CRN 76-05-1 	Biological Study (BIOL); Pharmacological Activity (PAC); Preparation (PREP); Synthetic Preparation (SPN); Therapeutic Use (THU); Uses (USES) prepn. of benzoxaborole derivs. useful for treating bacterial infections
1364683-03-3 *(Cmpd. 3)* 1-Propanol, 3-[[3-(aminomethyl)-4-chloro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, hydrochloride (1:1)		Biological Study (BIOL); Pharmacological Activity (PAC); Preparation (PREP); Synthetic Preparation (SPN); Therapeutic Use (THU); Uses (USES)

Summary Record export with Hit Structures

Classic STN (STN Express)

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

Hit Structures:

1364682-96-1 *(Cmpd. 2)* 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  CM 2 CRN 76-05-1 	RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) preparation of benzoxaborole derivs. useful for treating bacterial infections
1364683-03-3 *(Cmpd. 3)* 1-Propanol, 3-[[3-(aminomethyl)-4-chloro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-		RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

Summary Record export with Hit Structures

STNext

3. **Basic Patent Number:** **WO2012033858A2**

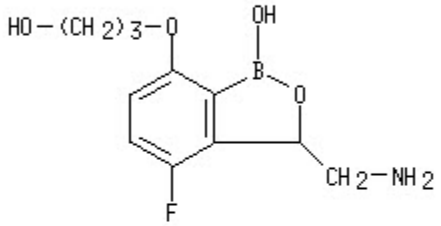
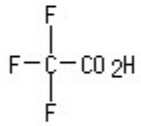
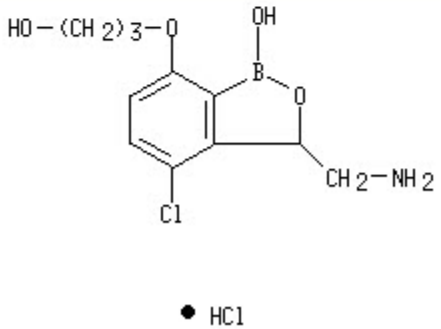
Title: Boron-containing small molecules

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

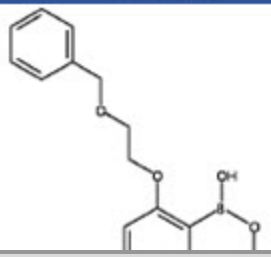
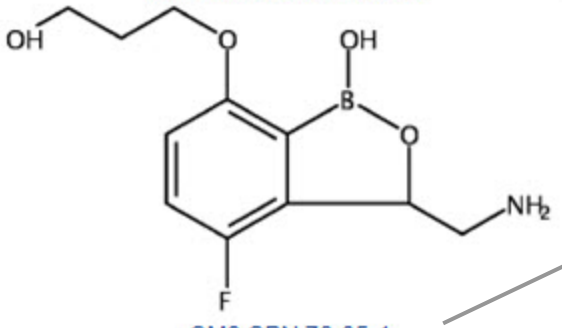
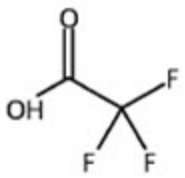
Hyperlinks: Source | WO2012033858A2

Hit Structures:

1364682-96-1 *(Cmpd. 2)* 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  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
1364683-03-3 *(Cmpd. 3)* 1-Propanol, 3-[[3-(aminomethyl)-4-chloro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, hydrochloride (1:1) (CA INDEX NAME)		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

Or, structure oriented “Index of Hit Structures”

Index of Hit Structures

	Substance	Structure	
1	1655492-02-6 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-(nitromethyl)-7-[2-(phenylmethoxy)ethoxy]-		pr… 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)	 CM2 CRN 76-05-1 	prepn. of benzoxaborole derivs. useful for treating bacterial infections *Reference 3*

Structures with annotations

Each hit substance identified

Links to references for each structure

Multiple images (continuation) or mixtures

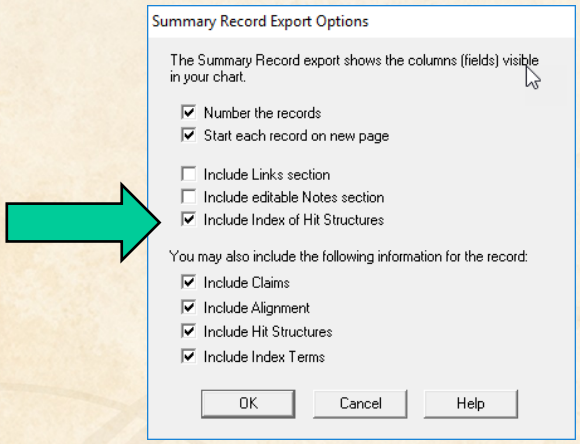
Importing transcripts with hit structures

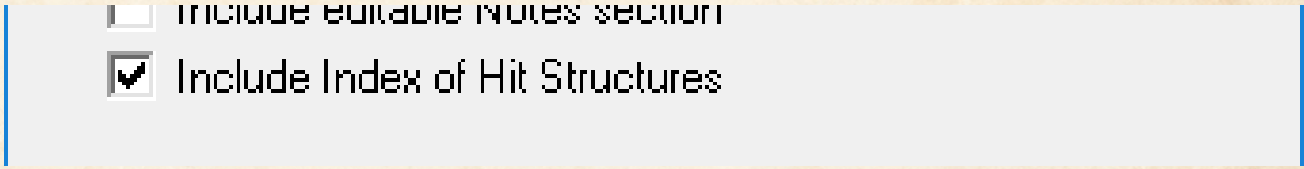
New STN: BizInt export – must include both REGISTRY and CAplus records in export
http://www.bizint.com/support/create/newstn_hitstr.php

Classic STN: Using STN Express, display HITSTR, save transcript as RTF.
If transcript opens in Word DO NOT SAVE!

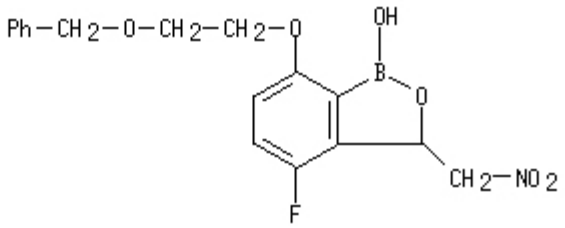
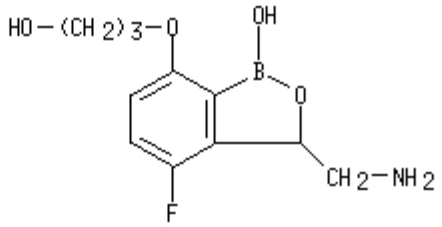
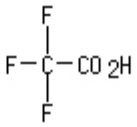
STNext: Display HITSTR.
Turn off enhanced display. Save as RTF.

Option: Index of Hit Structures

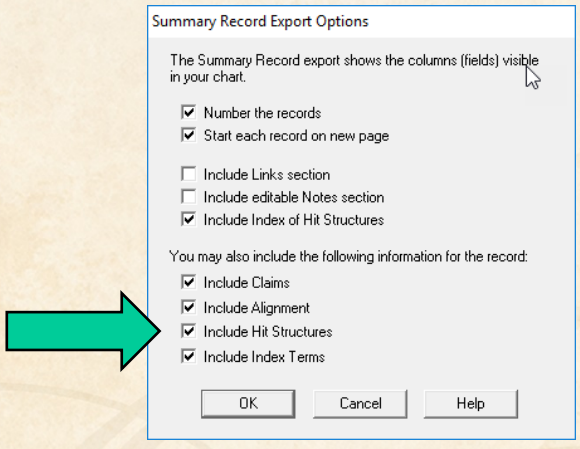


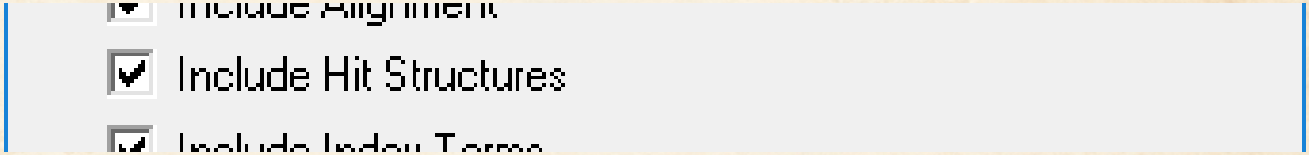


Index of Hit Structures

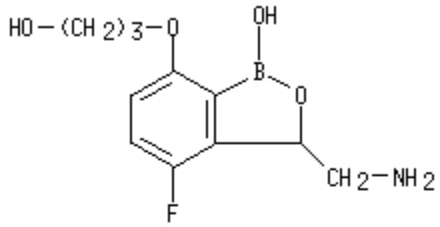
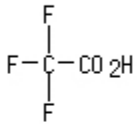
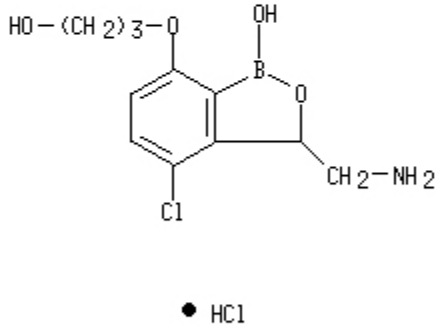
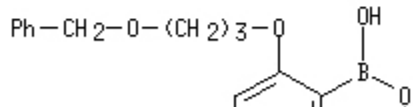
	Substance	Structure	Reference
1	1655492-02-6 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-(nitromethyl)-7-[2- (phenylmethoxy)ethoxy]- (CA INDEX NAME)		prepn. and anti-mycobacterial activity of benzoxaborole compds. Reference 1 prepn. and biol. applications of tricyclic benzoxaborole compds. Reference 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  CM 2 CRN 76-05-1 	prepn. of benzoxaborole derivs. useful for treating bacterial infections Reference 3

Option: Hit Structures

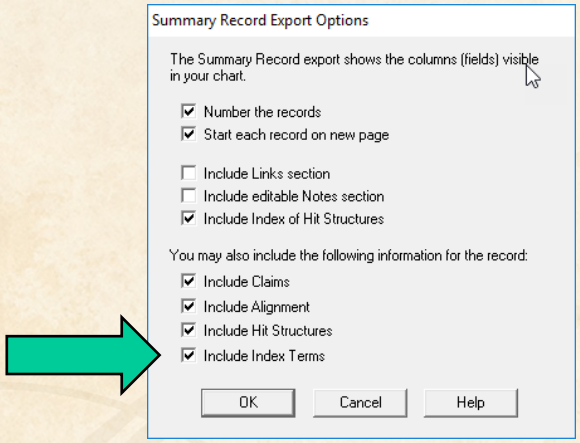


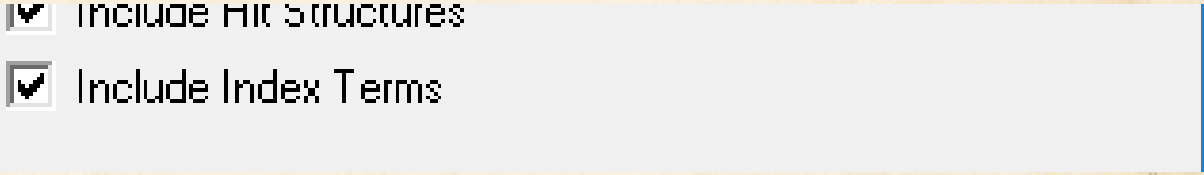


Hit Structures:

1364682-96-1 *(Cmpd. 2)* 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  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
1364683-03-3 *(Cmpd. 3)* 1-Propanol, 3-[[3-(aminomethyl)-4-chloro-1,3-dihydro-1-hydroxy-2,1-benzoxaborol-7-yl]oxy]-, hydrochloride (1:1) (CA INDEX NAME)		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
1364684-69-4 *(Cmpd. 4)* 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-		RL: RCT (Reactant); 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)

Create reports integrating key IP data…

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

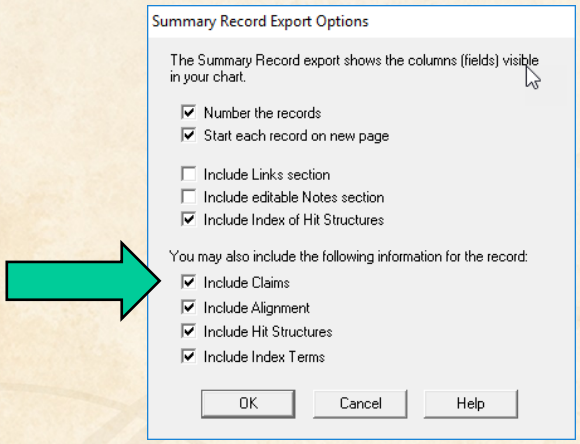
	Title	Database	Patent Family			Family Status				Probable Assignee	Sequence Locations			
			Patent	Kind	Date	Pub No.	State	Status	Expiry		Seq. ID Number	% Identity	Length	Location
1.	Modulating expression of a target nucleic acid comprises providing to the cell a guide RNA including a transcriptional 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 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	US 20140356956 A1 US 9267135 B2	ALIVE ALIVE	PENDING GRANTED	2034-06-04 2034-06-04	PRESIDENT AND FELLOWS OF HARVARD COLLEGE	US20140356959-0001 US20140356956-0001	100.00 100.00	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				1.3 1.4
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	A1 A A	2015-05-14 2015-05-14 2015-12-10	WO 201570193 A1 US 20150132263 A1 US 20150353901 A1	ALIVE ALIVE ALIVE	PENDING PENDING PENDING	2034-11-11 2034-11-11 2034-11-11	RADIANT GENOMICS INC	US20150132263-0002 US20150353901-0002	100.00 100.00	1368 1368	claim: 19; 20 claim: 19; 20
	2.1 DWPI		2.5 Patbase			2.6 FAMPAT				2.5 Patbase				2.3 2.4

Integrate Hit structures with 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)

Option: Claims + Hit Structures



Claims:

US2016251380A

1. A compound having a structure as shown in Formula II:

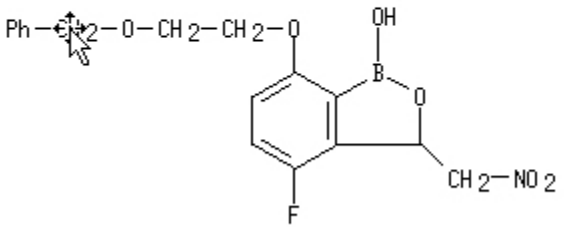
[FTIMG=86863146]
wherein X is selected from fluoro, chloro, bromo or iodo and R1 and R2 are each independently selected from H, -CH3, -CH2CH3, -CH2CH2CH3, and -CH(CH3)2; or a salt thereof.

2. A compound according to claim 1 or a salt thereof, wherein X is chloro or bromo.

58. A method according to claim 57, wherein the mycobacterial infection is a Mycobacterium tuberculosis infection.

59. A method according to claim 57, wherein the animal is a human.

t Structures:

1655492-02-6 *(Cmpd. 1)* 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-(nitromethyl)-7-[2-(phenylmethoxy)ethoxy]- (CA INDEX NAME)		RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) prepn. and biol. applications of tricyclic benzoxaborole compds.

Integrate Hit structures with 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)

Link sequence results with hit structures

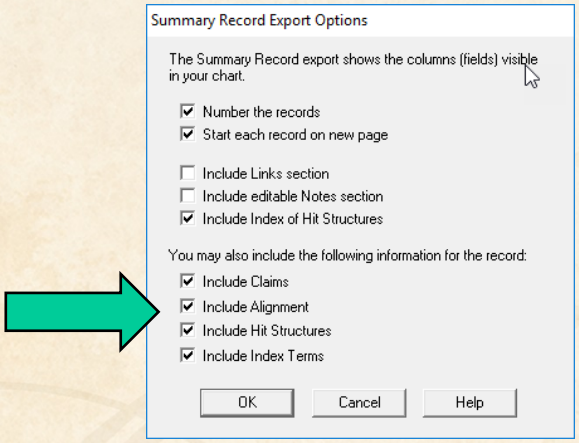
Follow Cookbook recipe to create a summary of sequence hits for each

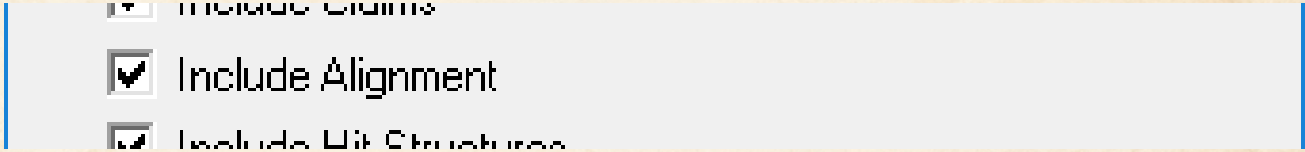
1.	Title:	**Selective high-affinity polydentate ligands and methods of making such**
	Database:	GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins GQPAT Gold+ Proteins Chemical Abstracts Chemical Abstracts
	Organism Species:	Homo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

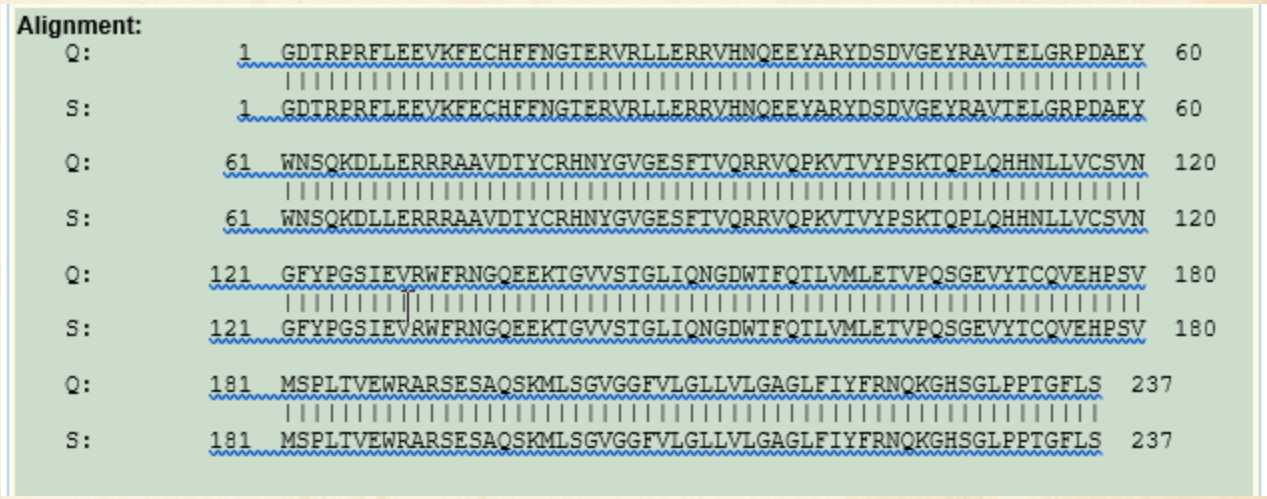
Sequence Summary:

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)

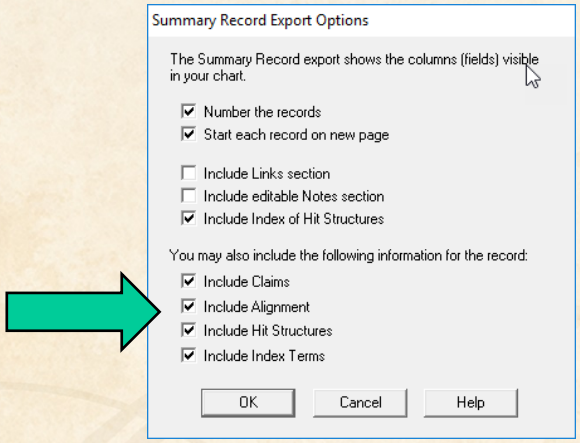
Option: Alignments + Hit Structures

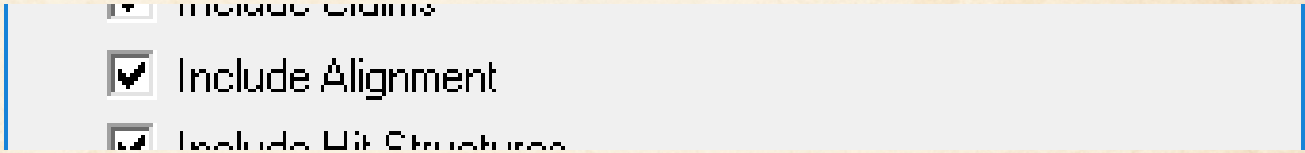






Option: Alignments + Hit Structures



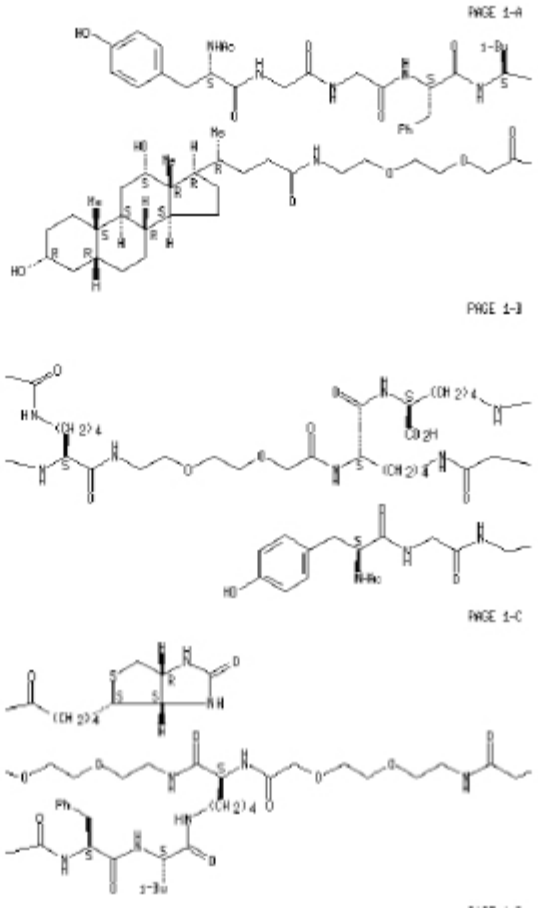


Hit Structures:

1045703-23-8 *(Cmpd. 1)*

L-Lysine, N2,N6-bis[N6-(N-acetyl-L-tyrosylglycylglycyl-L-phenylalanyl-L-leucyl)-N2-[2-[2-[2-[[(3 oxocholan-24-yl]amino]ethoxy]ethoxy]acetyl]-L-lysyl-2-[2-(2-aminoethoxy)ethoxy]acetyl]-L-lysyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H- thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]- (CA INDEX NAME)

Absolute stereochemistry.



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

Integrate Hit structures with 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…

1. **Title:** **Heterocyclic derivatives as eIF4A inhibitors and their preparation**

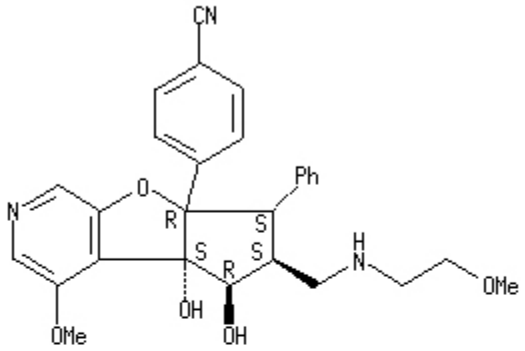
Accession Number: 2017:1085458

Hit Structures:

2098192-11-9 *(Cmpd. 1)*

INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (-).



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

2. **Title:** **Heterocyclic derivatives as eIF4A inhibitors and their preparation**

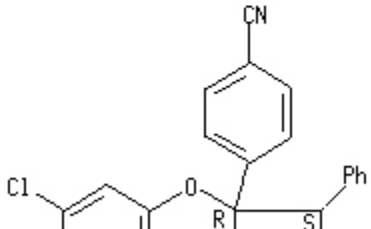
Accession Number: 2017:1085457

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

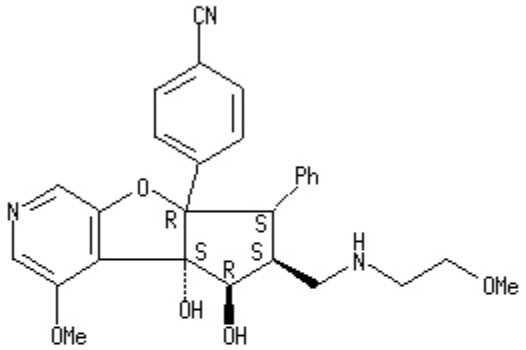
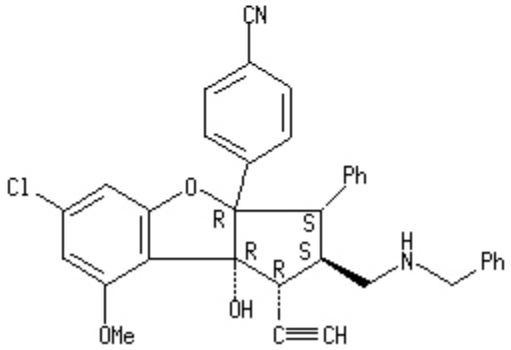
Group Mega-TAN records

Simply send to Reference Rows and export!

1. **Title:** **Heterocyclic derivatives as eIF4A inhibitors and their preparation**

Accession Number: 2017:1085458; 2017:1085457

Hit Structures:

2098192-11-9 *(Cmpd. 1)* INDEX NAME NOT YET ASSIGNED	Absolute stereochemistry. Rotation (-). 	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
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

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

2018 is the Year of the Dog!

狗

Thank you...

Questions???

bizint.com/slides