Software for Business Intelligence

BizInt Smart Charts

Patents & IP Sequences | Clinical Trials | Drug Pipelines

Workshop - Proposed MARPAT support in BizInt Smart Charts for Patents

3 June 2020, incorporating feedback from the workshop

John Willmore, VP Product Development

Diane Webb, President

www.bizint.com

Notes from the Workshop

- Thank you for your participation and for all the excellent feedback.
- These slides have been updated to incorporate some clarifications and additional ideas.
- New content is in purple text.

Background

- Customers have been requesting MARPAT support in BizInt Smart Charts for Patents for several years.
- One customer just gave us a detailed design for what they would like to see.
- *To implement MARPAT support, we need a BizInt export on STNext.*

Purpose of today's workshop

- Present proposed MARPAT support in BizInt Smart Charts for Patents.
- Get your feedback – would you find this valuable?
- If so, encourage you to contact STN!

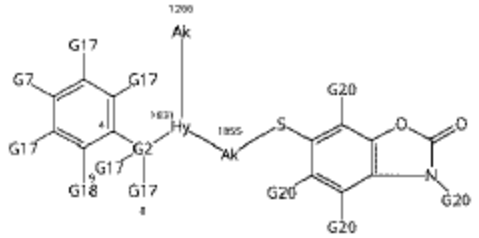
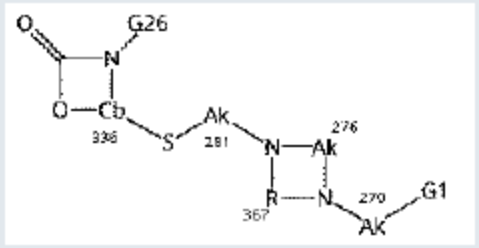
Our Ask

- File format problems continue to be our #1 support issue on STN
- Please ask CAS/STN to implement a BizInt export format on STNext
- This is an export format, like RTF
- We will communicate specifics to CAS/STN
- Everything that follows in this presentation depends on getting a BizInt export in place on STNext

Today's Topics

- Display Formats
- Presentation in Charts
- Image quality
- Presentation in Index of Hit Structures
- Your feedback

Current Display (Version 5.3)

	Title	Inventor(s)	Patent Assignee	Patent Family			Priority Date	Graphic Information
				Patent	Kind	Date		
1	**Pyrrolopyridine derivatives as inhibitors of the menin-MLL interaction and their preparation**	Cacatian, Salvacion Claremon, David A. Dong, Chengguo Fan, Yi Jia, Lanqi Lotesta, Stephen D. Singh, Suresh B. Venkatraman, Shankar Yuan, Jing Zheng, Yajun Zhuang, Linghang	Vitae Pharmaceuticals, Inc., USA	WO 2018053267	A1	20180322	2016-09-16	
				CA 3036987	A1	20180322		
				AR 109658	A1	20190109		
				AU 2017326006	A1	20190321		
				IL 265028	A	20190430		
				BR 112019005030	A2	20190618		
				MX 2019003091	A	20190708		
				EP 3512850	A1	20190724		
				KR 2019111008	A	20191001		
				CN 110325533	A	20191011		
				JP 2019529421	T	20191017		
				IN 201927007880	A	20190802		
				US 20190202830	A1	20190704		
2	**Neuroactive compounds comprising NMDA receptor modulators and methods of use for treating sterol synthesis disorders or sterol deficiency disorders**	Quirk, Michael C. Doherty, James J. Martinez Botella, Gabriel	Sage Therapeutics, Inc., USA	WO 2016057713	A1	20160414	2014-10-07	
				CA 2963938	A1	20160414		
				AU 2015330906	A1	20170427		
				IL 251505	A	20170529		
				KR 2017065637	A	20170613		
				EP 3204011	A1	20170816		
				JP 2017530982	T	20171019		
				CN 107405352	A	20171128		
				BR 112017007053	A2	20180619		
				MX 2017004684	A	20170630		
				US 20170304321	A1	20171026		
				ZA 2017002545	A	20190626		
				IN 201717014604	A	20170915		

MARPAT Display Formats

- BIB AB FQHIT
  BIB AB QHIT
  BIB ABS FQHIT
  …

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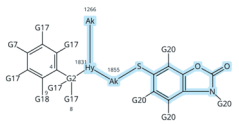
d bib ab fqhit 1-

YOU HAVE REQUESTED DATA FROM 14 ANSWERS - CONTINUE? Y/(N):y


L3   ANSWER 1 OF 14  MARPAT  COPYRIGHT 2020 ACS on STN
AN   168:367011  MARPAT  Full-text
TI   Pyrrolopyridine derivatives as inhibitors of the menin-MLL interaction and
     their preparation
IN   Cacatian, Salvacion; Claremon, David A.; Dong, Chengguo; Fan, Yi; Jia,
     Lanqi; Lotesta, Stephen D.; Singh, Suresh B.; Venkatraman, Shankar; Yuan,
     Jing; Zheng, Yajun; Zhuang, Linghang
PA   Vitae Pharmaceuticals, Inc., USA
SO   PCT Int. Appl., 285pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND  DATE       APPLICATION NO.          DATE
     ------------------  ----  ---------  -----------------------  ---------
PI   WO 2018053267       A1    20180322   WO 2017-US51780          20170915
     CA 3036987          A1    20180322   CA 2017-3036987          20170915
     AR 109658           A1    20190109   AR 2017-102556           20170915
     AU 2017326006       A1    20190321   AU 2017-326006           20170915
     IL 265028           A     20190430   IL 2017-265028           20170915
     BR 112019005030     A2    20190618   BR 2019-112019005030     20170915
     MX 2019003091       A     20190708   MX 2019-3091             20170915
     EP 3512850          A1    20190724   EP 2017-772585           20170915
     KR 2019111008       A     20191001   KR 2019-7010730          20170915
     CN 110325533        A     20191011   CN 2017-80063763         20170915
     JP 2019529421       T     20191017   JP 2019-514787           20170915
     IN 201927007880     A     20190802   IN 2019-27007880         20190228
     US 20190202830      A1    20190704   US 2019-16333852         20190315
PRAI US 2016-62395618          20160916
     WO 2017-US51780           20170915
OS   CASREACT 168:367011; CASFORMULINS 2018:519257
AB   The invention is directed to pyrrolopyridine derivs. of formula I as
     inhibitors of the interaction of menin with MLL and MLL fusion proteins,
     pharmaceutical compns. contg. the same, and their use in the treatment of
     cancer and other diseases mediated by the menin-MLL interaction.  Compds.
     of formula I wherein A is C6-10 aryl, 5- to 14-membered heteroaryl, C3-14
     cycloalkyl, 4- to 14-membered heterocycloalkyl; U is CRa and N; Ra is H,
     halo, CN, OH, etc.; V and W are independently N and C; Y is CRb, CO and
     CS; Rb is H, halo, CN, OH, C1-4 alkyl, etc.; dashed bonds are
     independently single and double bond; X is F and Cl; Z is halo, C1-6
     alkyl, C2-6 alkenyl, CN, NO2, etc.; n and m are independently 0 and 1; p
     is 0, 1, 2 and 3; q is 0, 1 and 2; L is C1-6 alkylene and (C1-4
     alkylene)0-4-Q-(C1-4 alkylene)0-1; Q is O, SO, SO, SO2, CO, etc.; Cy is
     (un)substituted C6-10 aryl, (un)substituted C3-18 cycloalkyl,
     (un)substituted 5- to 14-membered heteroaryl, and (un)substituted 4- to
     18-membered heterocycloalkyl; R1 is H, halo, C1-6 alkyl, CN, NO2, C1-4
     haloalkyl, etc.; R2, R3, R4 and R5 are independently H, halo, C1-6 alkyl,
     C1-4 haloalkyl, C1-4 cyanoalkyl, C2-6 alkenyl, etc.; and pharmaceutically
     acceptable salts thereof, are claimed.  Example compd. II was prepd. by
     hydrolysis of tert-Bu 4-(1-(4-fluoro-2-(isopropyl(methyl)carbamoyl)phenyl)-
     1H-pyrrolo[2,3-c]pyridin-3-yl)piperidine-1-carboxylate; the resulting
     5-fluoro-N-isopropyl-N-methyl-2-(3-(piperidin-4-yl)-1H-pyrrolo[2,3-
     c]pyridin-1-yl)benzamide underwent reductive alkylation with benzaldehyde
     to give compd. II.  The invention compds. were evaluated for their
     menin-MLL interaction inhibitory activity.  From the assay, it was detd.
     that compd. II exhibited EC50 value of < 100 nM.

  MSTR 1A Assembled



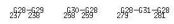
1266: carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple
bonds> (opt. substd.)
1831: heterocycle <containing up to 14 atoms, 1 or more heteroatoms, zero or
more N, zero or more O, zero or more S (no other heteroatoms), 0 or more double
bonds> (opt. substd. by 1 or more G8)
1855: alkylene <containing 1 or more C> (opt. substd.)
Patent location:          claim 1
Note:                     or pharmaceutically acceptable salts
Note:                     substitution is restricted
Note:                     additional derivatization also claimed

  MSTR 1A

G1    = 216-11 217-7

G8    = carbon chain <containing 1-6 C,
        0 or more double bonds, 0 or more triple bonds>
        (opt. substd.)
G21   = 775

G25   = heterocycle <containing up to 14 atoms,
        1 or more heteroatoms, zero or more N, zero or more O,
        zero or more S (no other heteroatoms),
        0 or more double bonds> (opt. substd. by 1 or more G8)
G26   = 237-11 238-217  / 258-11 259-217  /
        279-11 281-217



G28   = alkylene <containing 1 or more C> (opt. substd.)
G30   = S
G32   = O
Patent location:          claim 1
Note:                     or pharmaceutically acceptable salts
Note:                     substitution is restricted
Note:                     additional derivatization also claimed

RE.CNT 3    THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
            ALL CITATIONS AVAILABLE IN THE RE FORMAT
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BIB AB
(Supported today)

Assembled Structure(s)

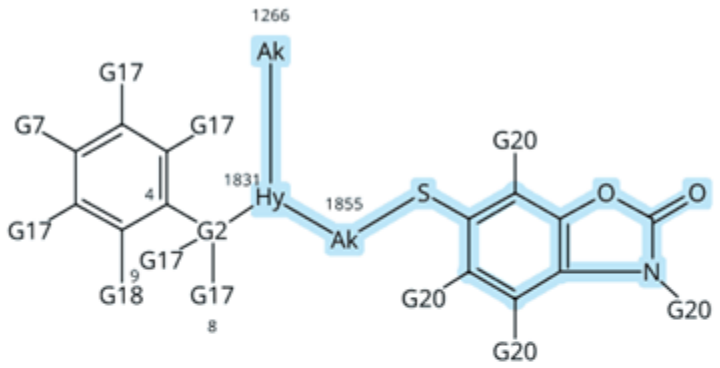
Unassembled Structure

Display Format Limitations

- Assembled structures only
- Unassembled structures will be ignored
  Suggestion: “Assembled structure not available” in the event of a hit structure without assembled structure
- Not sure whether QHITEXG format will work yet (are G-group descriptions text only vs. text + structures?)

Data Elements (Columns)

MSTR 1A Assembled



1266: carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.)
1831: heterocycle <containing up to 14 atoms, 1 or more heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms), 0 or more double bonds> (opt. substd. by 1 or more G8)
1855: alkylene <containing 1 or more C> (opt. substd.)
Patent location: claim 1
Note: or pharmaceutically acceptable salts
Note: substitution is restricted
Note: additional derivatization also claimed

Assembled Structure

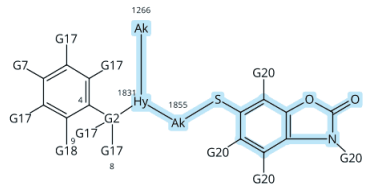
Node Annotations

Patent Location

Notes

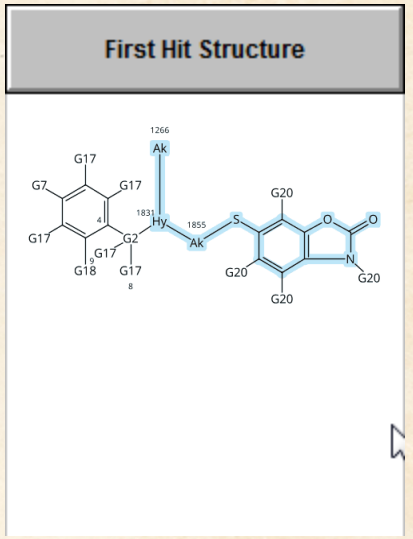
Proposed New Columns

MARPAT: Proposed New Fields

	Title	First Hit Structure	Patent Location	Node Annotations	Structure Notes
1	**Pyrrolopyridine derivatives as inhibitors of the menin-MLL interaction and their preparation**		claim 1	1266: carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.) 1831: heterocycle <containing up to 14 atoms, 1 or more heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms), 0 or more double bonds> (opt. substd. by 1 or more G8) 1855: alkylene <containing 1 or more C> (opt. substd.)	or pharmaceutically acceptable salts substitution is restricted additional derivatization also claimed

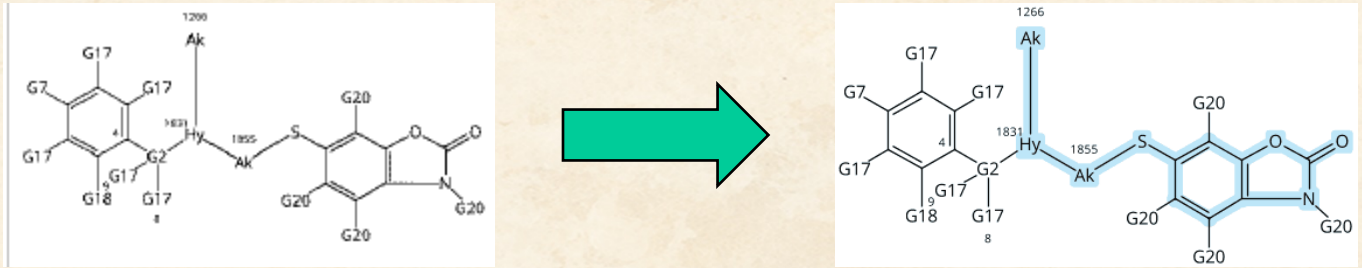
Proposed Column: First Hit Structure

- Add to both CAplus and MARPAT
- Shows first hit structure
- In addition to GI (Abstract Structure)
- Question from the workshop is how to display both CAPLUS and MARPAT hit structures
  - Separate columns?
  - Summarize rule in Reference Rows?



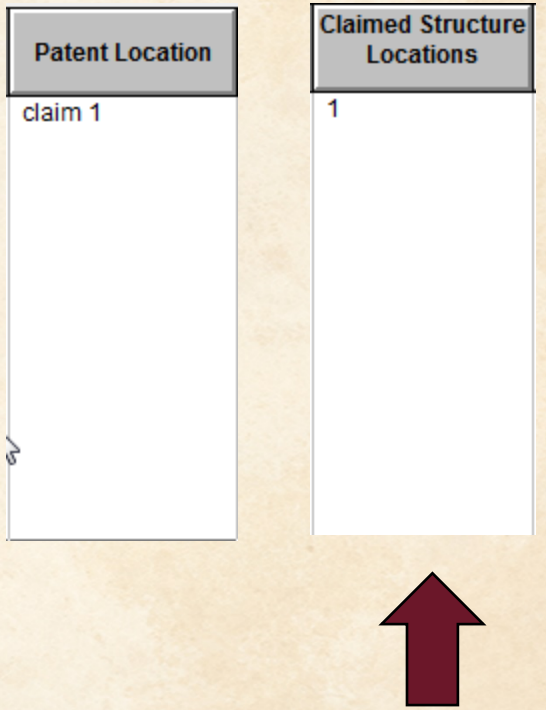
Structure Image Quality

- BizInt isn't handling the latest STNext structure displays well
- Improve resolution
- Support color hit indications ~~(option?)~~
- REGISTRY, CAPLUS, and MARPAT



Proposed Column: Patent Location

- Patent location for first hit structure (from structure annotations)
- Patent Location not limited to claims
- We could also capture a deduplicated list of claim numbers (only) from all hits in a record "Claimed Structure Locations"
- Would investigate whether it is possible to capture additional claim locations from Notes



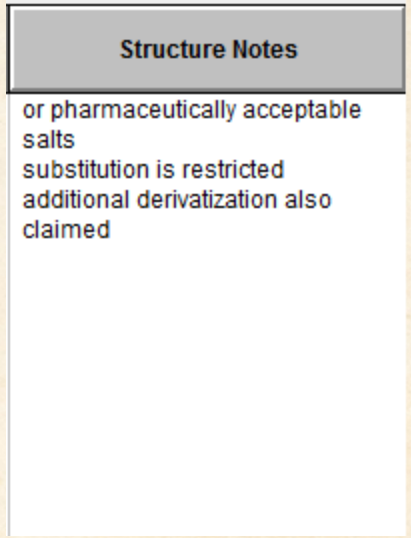
Proposed Column: Node Annotations

- List of node annotations from the first assembled hit structure, as paragraphs

Node Annotations
1266: carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.) 1831: heterocycle <containing up to 14 atoms, 1 or more heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms), 0 or more double bonds> (opt. substd. by 1 or more G8) 1855: alkylene <containing 1 or more C> (opt. substd.)

Proposed Column: Structure Notes

- List of notes from the first assembled hit structure, as paragraphs
- Includes Stereochemistry
- “Note:” prefixes removed



Proposed Column: Additional G-groups

- (Added based on workshop feedback)
- List of additional G-groups from QHITEXG display format

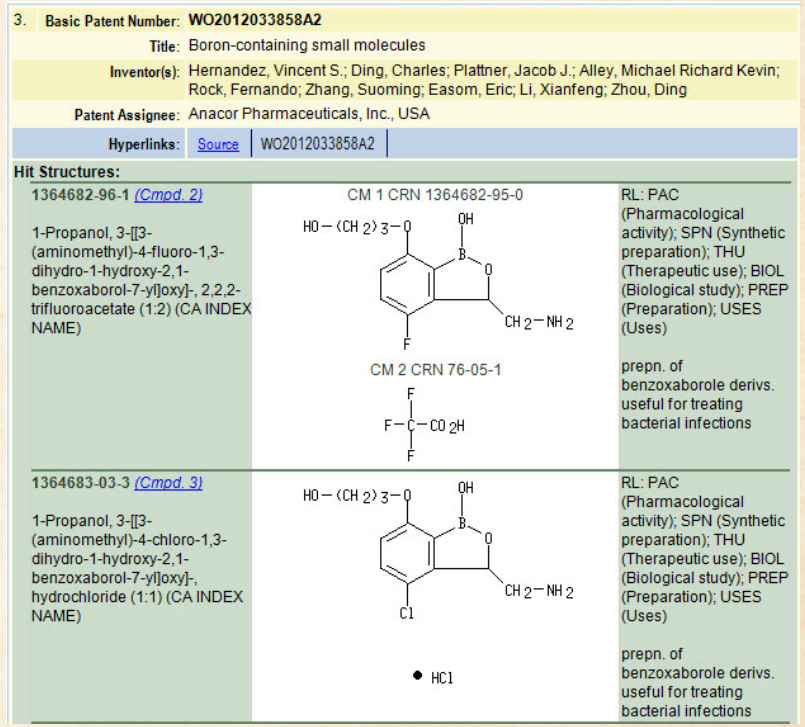
Additional G-groups
G1 = alkyl <containing 1-10 C> / any ring <containing zero or more N, zero or more O, zero or more S (no other heteroatoms), aromatic, 1-3 rings, including 5- or 6-membered rings> (opt. substd. by G7) / (Specifically claimed: Me / Ph (opt. substd. by G7)) / (Examples: Et / Pr-n / Pr-i / Bu-n / Bu-i / Bu-s / Bu-t) G3 = H / R

Proposed Column: Num Hit Structures

- (Added based on workshop feedback)
- A simple column with the number of hit structures for the reference.
- This would be available in both CAPLUS and MARPAT charts

Integrating MARPAT in the Index of Hit Structures

- Creating an equivalent to the CAPLUS hit structure display in summary records
- Lists all assembled hit structures and annotations under the reference
- In Reference Rows, a family could have both HITSTR and QHIT displays



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

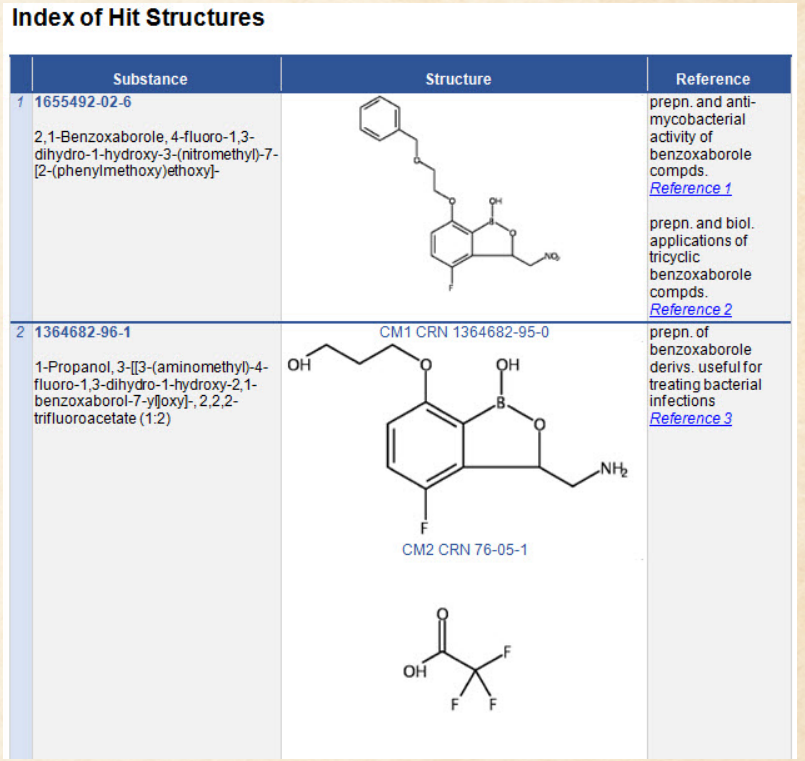
Hyperlinks: Source | WO2012033858A2

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)	• HCl	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

Integrating MARPAT in the Index of Hit Structures

- Index will be a structure list, rather than an index. Each structure to point to a single reference.
- ~~Is it possible to equate assembled hit structures from different famililes?~~
- ~~A simple difference in node numbering would result in image differences.~~

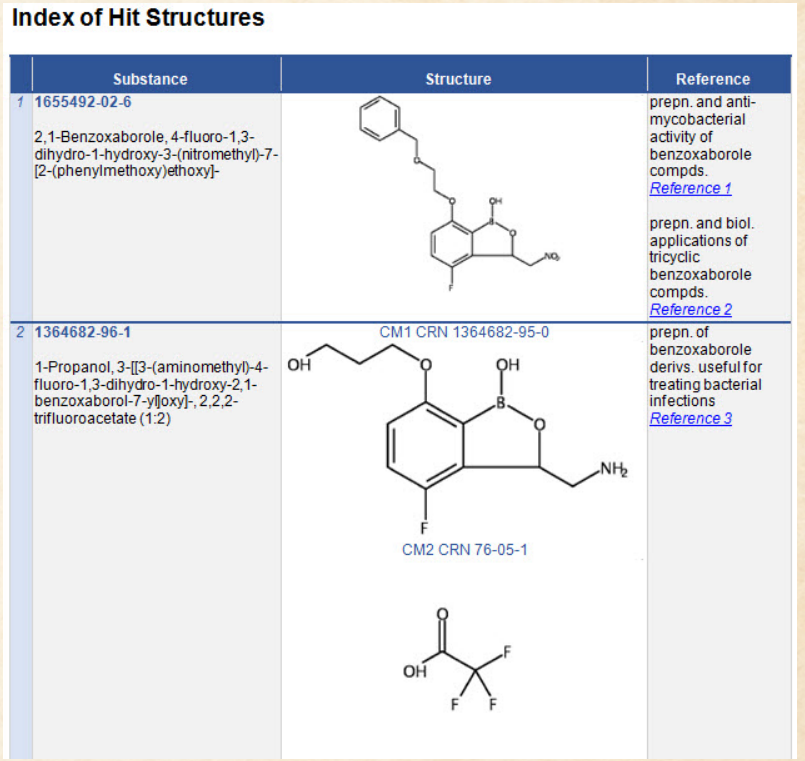


Index of Hit Structures

	Substance	Structure	Reference
1	1655492-02-6 2,1-Benzoxaborole, 4-fluoro-1,3-dihydro-1-hydroxy-3-(nitromethyl)-7-[2-(phenylmethoxy)ethoxy]-		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)	CM1 CRN 1364682-95-0 CM2 CRN 76-05-1	prepn. of benzoxaborole derivs. useful for treating bacterial infections *Reference 3*

Integrating MARPAT in the Index of Hit Structures (II)

- We envision this being a separate table from the CAPLUS hit structures index
- A similar presentation could be created for REGISTRY
- As with the existing Index of Hit Structures, this will be an optional display



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]-		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)	CM1 CRN 1364682-95-0 CM2 CRN 76-05-1	prepn. of benzoxaborole derivs. useful for treating bacterial infections Reference 3

Actions - You

- **Contact your STN Account Manager to request a BizInt export!**
- Send us sample transcripts of edge cases we need to worry about
- Feedback and suggestions

Actions - STN

- Implement a BizInt export option on STNext

Actions - BizInt

- Adjust STN parser to capture the assembled Markush and related data, skip all unassembled structure sections, populate new columns
- First hit structure column
- Improve STNext image quality
  - Full resolution images
  - Color highlights (Markush and Hit Structures)
- Add MARPAT support to Index of Hit Structures

Software for
Business Intelligence

BizInt Smart Charts

support@bizint.com

Feedback?